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TURBULENT DIFFUSION AND RIVER WASTE ASSIMILATIVE CAPACITY

Peter A. Krenkel

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Nashville, Tennessee

1 May 1964

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Turbulent Diffusion & River Waste Assimilative Capacity

Progress Report: 1 May 1962—1 May 1964

PETER A. KRENKEL

Technical Report Number 3
Sanitary & Water Resources Engineering
Department of Civil Engineering
Vanderbilt University
Nashville, Tennessee

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TURBULENT DIFFUSION AND RIVER WASTE ASSIMILATIVE CAPACITY

Progress Report: 1 May 1962 - 1 May 1964

Research Grant Number WP-328, Division of Water Supply and Pollution Control, U.S. Public Health Service

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SUMMARY

A brief review of current literature in both stream reaeration and the mixing process in inland waterways is presented. The analysis of turbulent diffusion parameters is elucidated and their application to water quality studies is described. The methodology utilized to determine the various mixing coefficients is outlined, and plans for the collection of pertinent mixing data both in the laboratory flume and in selected Tennessee rivers is depicted. The experimental flume and pertinent measuring instruments promulgated by this study are discussed and their application and potential to the research objectives are explained.

Functional relationships between the various mixing coefficients, the energy expenditure per unit mass of fluid and the reaeration coefficient are discussed and a rational basis for subsequent analysis is presented. It is demonstrated that the Kolmogoroff principle allows prediction of the longitudinal mixing coefficient from energy considerations and thus relates energy expenditure to reaeration.

The pulse testing technique as utilized by chemical engineers is elucidated and the application of this technique to the mixing problem is demonstrated.

Utilizing pulse testing methodology, the mathematical model depicting longitudinal mixing is tested and a new analysis of the pertinent parameters is presented.

TURBULENT DIFFUSION AND RIVER WASTE ASSIMILATIVE CAPACITY

Progress Report 1 May 1962 - 1 May 1964

Peter A. Krenkel

I. INTRODUCTION

1. Description of Investigations

The investigations described herein were initiated as a result of preliminary studies conducted in a one foot laboratory flume. These studies, which included a comprehensive review of available literature concerned with the mixing process in inland waterways and the aeration of water, demonstrated a need for a logical description of the mixing process and a paucity of field data which could be utilized in water quality studies.

Industrial communities situated in the proximity of large bodies of water, or with convenient access to such waters, ultimately dispose of their waste waters using these receiving waters as a diluent. Although there are cases where disposal by irrigation or evaporation of the waste water after the majority of the solids have been removed is mandatory, comparatively few large industrial communities in the United States do not use dilution as the predominant form of ultimate waste water disposal.

Wastes originating from a wide diversity of establishments, and widely varying in characteristics, ultimately depend on the natural process of purification effected by our rivers, streams, lakes, and harbors. These natural processes can be efficiently utilized only if the dilution process is aided by adequate natural mixing and dispersion of the waste waters after they have been introduced into the receiving waters.

It is obvious that an effective means of predicting the dispersion characteristics of a receiving water would enable achievement of optimum usage of the natural purification factors inherent to receiving water systems.

Also, since the mixing characteristics of a river must be related to its mass transfer characteristics, a descriptive system for turbulent diffusion should yield an insight into the mechanism by which oxygen is transferred into the water. Preliminary studies have resulted in a relationship between the longitudinal mixing coefficient and gas transfer into a turbulent liquid, thereby indicating a partial solution to the perplexing sanitary engineering problem of predicting the reaeration characteristics of a river.

Confirmation of the relationship established between turbulent diffusion and reaeration would allow waste assimilative capacity prediction by simply measuring the hydraulic and turbulent characteristics of the stream. Because hydraulic parameters are relatively unaffected by the biota, error induced by biological activity, which is inherent to previous methods for measuring the reaeration capacity, would be eliminated, thereby enabling a more accurate estimation of the stream's waste assimilative capacity.

The specific objectives of this investigation were as follows:

(1) To determine the applicability of the mathematical model describing turbulent diffusion with convection in open channel flow:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - \bar{u} \frac{\partial c}{\partial x} \qquad (1)$$

in describing the concentration gradients for a point or line source of waste contaminant in two-dimensional flow.

(2) To determine the relation between equation (1) and the conventionally defined eddy diffusivity, D_E :

$$\frac{\partial c}{\partial t} = D_E \frac{\partial^2 c}{\partial x^2} \qquad (2)$$

in a homogeneous turbulent field.

(3) To examine the methods of determination of these mixing coefficients in the model and to determine the practicability of these methods for field scale studies.

(4) To evaluate diffusion and longitudinal mixing coefficients for artificial and natural channels in terms of conventionally used hydraulic parameters.

(5) To correlate turbulent diffusion characteristics of natural streams to the reaeration capacity and thereby the waste assimilative capacity.

(6) Utilizing pulse testing techniques, to develop the frequency response characteristics of various streams under differing hydraulic conditions.

(7) To test the model and techniques developed as a result of these model studies on the prototype, i.e., field scale studies in a natural river.

Although these objectives appear to be quite optimistic, a logical solution to the overall mixing process in inland waterways requires that each be subjected to analysis. Also the experimental procedures may be designed such that information pertinent to each phase of the investigation will be obtained.

2. Organization of the Report

The progress report contained herein is essentially arranged in two

sections, the first containing a brief description of the research status of mixing and reaeration, and the second, indicating the accomplishments of this investigation during the report period.

Also, an appendix is included which contains a list of publications supported in whole or in part by this grant, a description of the professional staff involved, and a paper pertinent to the discussion of frequency response techniques developed.

3. Present Status of Research

a. Mixing Analysis:

(1) Eddy Diffusion

Oceanographers and meteorologists have long used the analogy between diffusion of matter on a microscopic scale and the spread of a tracer material on a macroscopic scale to describe turbulent mixing in the ocean and in the atmosphere. This process can be described by Fick's second law, which is

$$\frac{\partial C}{\partial t} = D_E \frac{\partial^2 C}{\partial x^2} \qquad (2)$$

in which C is the concentration, t is the time, x is the distance, and D_E is the eddy diffusion coefficient. Although the analogy has been subjected to question, one can find much experimental evidence of the molecular diffusion process on a macro-scale as applied to the spread of tracers in a turbulent field both in the ocean and in the atmosphere. An excellent summary of the process, including experimental verification of the analogy, can be found in a report by Harlemann et. al. (1).

Although equation 2 has been used successfully in numerous diffusion investigations, it should be recognized that in the case in question, (that is, in open channel flow), use of this mathematical model may result in erroneous conclusions.

The concentration gradient predicted by this model may be in error because of the neglected mass transport caused by the convective velocity. Also, the eddy diffusion coefficient as previously defined describes mixing at a point in the flow, and as such may not be the parameter desired to denote mass transfer in a stream section. To predict the mixing characteristics of a river section using equation 2, it would be necessary to determine the eddy diffusion coefficient at numerous points and then use an appropriate averaging technique to obtain the overall description of mixing in the section under consideration. As shown subsequently, this averaging process is performed automatically when the longitudinal mixing coefficient is used.

(2) Longitudinal Mixing Coefficient

Consider an experiment in which an instantaneous dose of tracer has been injected into an open channel where the water is flowing at a mean velocity, $\bar{u}$. If samples are taken with respect to time at a station downstream from the point of injection, the flow pattern will typically follow equation 1:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - \bar{u} \frac{\partial C}{\partial x} \qquad (1)$$

which is the general differential equation describing the mixing process of the injected tracer. A solution to this equation is

$$C = \frac{M}{A(4\pi D_L t)^{1/2}} \exp\left[- \frac{(x - \bar{u}t)^2}{4D_L t} \right] \qquad (3)$$

where M is the weight of injected tracer material, A is the cross sectional area and x is the distance downstream from the point of injection.

Equation 3 has been found to describe very closely the temporal distribution

of an instantaneously injected tracer, and is similar to the equation developed by Taylor (2) (3), partly by intuition. Examination of this equation shows it to be representative of the normal error curve if the tracer distribution with distance is observed at a particular time. Normally, in experiments of the type described, the tracer is instantaneously injected and the concentration distribution as a function of time is observed at a fixed station downstream. Obviously, because the exponential denominator in equation 3 is no longer constant in this case, one would expect to obtain a skewed time-concentration distribution. This observation has been made by Taylor who states that the asymmetry should be negligible when the observation point is greater than 100 pipe diameters downstream from the point of tracer injection. A physical explanation of the skewness may lie in the fact that diffusion is taking place while the tracer cloud is passing the observation point.

It should be noted that when a significant laminar sublayer exists, the time-concentration curve may not follow equation 3 because of the slow release of tracer particles from the sublayer itself. This could explain the extremely long tails that are obtained in tracer tests conducted in sedimentation basins, for in this case it is highly probable that a significant laminar sublayer is present.

Elder (4), in an attempt to explain the deviation of the observed time-concentration curve that is sometimes obtained from the theoretically predicted distribution, proposed the following mechanism. The observed time-concentration curve is considered to be composed of two components - the primary one corresponding to tracer that is carried in the turbulent flow regime, and the secondary one resulting from the slow release of tracer existing in the viscous sublayer. Elder considered that particles contained in the laminar layer could only be released

to the turbulent portion of the stream via the process of molecular diffusion.

By manipulation of equation 3 it is possible to obtain the solution given by Levenspiel (5) in his investigations of the longitudinal mixing process:

$$\frac{C\,V}{V_t} = \frac{1}{\left[\frac{4\pi Qt D_L}{V\,\bar{u}\,L}\right]^{1/2}} \exp\left[-\left(1-\frac{Qt}{V}\right)^2 \Big/ \frac{4\,Qt\,D_L}{V\,\bar{u}\,L}\right] \qquad (4)$$

in which V is the volume of flow section considered, V_t is the volume of tracer injected if at unit concentration, and L is the length of flow section in question. Levenspiel showed that when $D_L/\bar{u}L$, which is the reciprocal of the Peclet number, is less than about 0.01, the time-concentration curve should be approximately normal because of the short time allowed for diffusion of the tracer cloud to occur while passing the point of observation.

Because the time-concentration distribution is usually obtained when performing experiments of the type described, it is convenient to determine the mean stream velocity directly from the observed curves. The question then arises as to what point on the curve most accurately represents the mean flow through time or velocity. Experiments by Allen and Taylor (6) indicate that this point lies on the peak or maximum concentration of tracer occurring on the flow-through distribution. Although this has been substantiated by other investigators, in some instances it appears that the centroid of the time-concentration distribution more nearly corresponds to the mean stream velocity. It is quite possible that the apparent discrepancy can be explained in terms of the turbulence intensity existing in the conduit. In cases where a significant boundary layer exists, the peak of the curve may not correspond to the mean flow-through time, and the time concentration distribution does not follow equation 3. However, if the phenomenon

is truly represented by the mathematical model presented herein, examination of the model shows that the mean velocity must correspond to the modal or peak value of the flow-through curve. The actual time represented when the concentration is a maximum can be found by differentiating equation 3 and equating to zero. The resulting expression for the time at maximum concentration is

$$t_{max} = \frac{-D_L \pm \left[D_L^2 + \bar{u}^2 x^2\right]^{1/2}}{\bar{u}^2} \qquad (5)$$

It is seen that the time of maximum concentration does not correspond to the modal concentration; however, when $D_L \ll \bar{u}\, x$, the time of occurrence of the peak is close to the mean detention time and, in this case, use of the modal concentration can be justified. It can also be shown that the centroid of the flow-through curve does not truly represent the mean detention time. Integrating the formulation for the centroid results in the following expression for the time represented by the centroid,

$$t_c = \frac{2D_L}{\bar{u}^2} + \frac{x}{\bar{u}} \qquad (6)$$

(3) Determination of Longitudinal Mixing Coefficient

The determination and subsequent calculation of the longitudinal mixing coefficient can be accomplished using several procedures; however, as shown, certain inaccuracies are inherent in several of the methods available.

Probably the most common source of error in tracer tests of the type described is caused by non-instantaneous injection of the tracer material into the flow stream. For determination of the longitudinal mixing coefficient in rivers where the process follows equation 3, this error can be substantially eliminated as

follows: It is seen that when the concentration-time curve is at a maximum the value of $(x - \bar{u}\, t)$ in Equation 3 must be zero. Therefore, at any two points downstream from the point of injection

$$C_1 = \frac{M}{A\,(4\pi\, D_L t_1)^{1/2}}$$

and

$$C_2 = \frac{M}{A\,(4\pi\, D_L t_2)^{1/2}}$$

Squaring and subtracting one expression from the other,

$$(C_1^2 - C_2^2) = \frac{M^2}{A^2 4\pi D_L t_1} - \frac{M^2}{A^2 4\pi D_L t_2}$$

from which

$$D_L = \frac{M^2}{4\pi\, A^2\, (C_1^2 - C_2^2)} \frac{t_2 - t_1}{t_2 t_1} \qquad (7)$$

An appropriate procedure, then, would be to introduce the tracer as quickly as possible in a manner that insures maximum mixing at the point of injection, and then obtain the time-concentration distribution at two stations downstream from the point of injection of tracer. The mixing coefficient can then be determined from the maximum concentrations. For fairly uniform channels, the determination of the cross-sectional area should present no problem; however, for ill-defined channels a graphical integration of the cross-sectional area may be necessary.

Writing Equation 3 in logarithmic form,

$$\log Ct^{1/2} = \log \frac{M}{A\,(4\pi D_L)^{1/2}} - \frac{(x - \bar{u}t)^2}{4 D_L t} \log e \qquad (8)$$

it is seen that by plotting $\log Ct^{1/2}$ versus $(x-\bar{u}t)^2/t$, the slope of the resulting straight line will be $\log e/4D_L$, from which D_L can be easily found. An advantage of this method is that the actual concentration of tracer material need not be known, thereby allowing the use of conductimetric or photometric instruments without tedous calibration procedures. This method is ideal for long uniform channels; but, as noted by Parker (7), in cases of highly irregular flow boundaries some difficulty may arise in determining the "line of best fit" of the observed data.

Using the equation for the standard deviation from Wilks (8),

$$\sigma^2 = {}_a\int^b x^2 f(x)\,dx - \left[{}_a\int^b x\, f(x)\,dx\right]^2 \qquad (9)$$

Levenspiel (5), assuming that $x = Qt/V$, $f(x)$ = Equation 3, and integrating from $a = 0$ to $b = \infty$, obtained

$$D_L = \frac{\bar{u}\, L}{8} \left(\sqrt{8\sigma^2 + 1} - 1\right) \qquad (10)$$

To obtain the variance of the time-concentration curve, Equation 9 is modified by replacing the integrals by finite sums and introducing the observed concentration readings. Thus,

$$\sigma_t^2 = \frac{\Sigma t^2 C}{\Sigma C} - \left[\frac{\Sigma tC}{\Sigma C}\right]^2 \qquad (11)$$

in which the summation is taken over all uniformly spaced readings, and

$$\sigma_t^2 = \left[\frac{V}{Q}\right]^2 \sigma^2 \tag{12}$$

This method does not require knowledge of absolute concentrations and, in addition, involves no subjectivity with respect to a "line of best fit." For these reasons, and because of the relative ease of calculation involved, this procedure will probably give the best practical results for determination of the mixing coefficient.

Assuming a normal distribution, Taylor (2) has shown that the mixing coefficient can be found from

$$D_L = \frac{X_{1/2}^2}{4t \log 2} = \frac{\bar{U}^3 t_{1/2}^2}{4x \log 2} \tag{13}$$

in which X is the length of conduit from injection point to observation point, $2X_{1/2}$ is the mean length of conduit containing fluid of concentration greater than one-half the maximum, and $2t_{1/2}$ is the time during which the concentration is greater than one-half the maximum. Because this formulation involves some subjectivity in determining the parameters involved, it probably will not be as accurate as the method outlined by Levenspiel; however, the relative ease of calculation involved allows Equation 13 to be used as a check on more complicated calculations.

(4) Determination of Eddy Diffusion Coefficient

As with the longitudinal mixing coefficient, several procedures are commonly used for its determination. Orlob (9) used the Einstein equation:

$$D_Z = \frac{1}{2} \frac{d(\sigma_Z)^2}{dt} \tag{14}$$

where D_z is the lateral coefficient of eddy diffusion, t denotes time, and σ_z represents the standard deveiation of the lateral displacement from the mean position of a statistically significant number of eddies. In a turbulent stream, the eddy motions were traced by point introduction of particles of polyethelene having a specific gravity slightly less than water, and collecting them in a manner such that statistical analysis of the particle positions could be performed. The particle distribution was then found for several distances downstream from the point of injection and equation 14 was utilized to determine the diffusion coefficient.

Pien (10), also utilizing the formulations of Taylor, determined the lateral and vertical diffusion coefficients using a steady state introduction of tracer material and measuring concentration changes with distance. Both photographic and chemical means were utilized in this investigation and the results demonstrated the variability of the diffusion coefficient with depth which indicates the desirability of using the longitudinal mixing coefficient as a measure of turbulent mixing. It should also be noted that a most convenient method of measuring the "scale" or mixing length of the diffusion process was devised, and that it also was found to vary with depth.

Other notable investigations yielding methods for the diffusion coefficient determination include the work of Richardson (11) who utilized a photometric measuring technique, and Elder (12) who traced the movement of droplets of permanganate introduced onto the water surface. Both of these investigations utilized the basic equations of diffusion as proposed by Taylor; however, the extremely short length of channel used by Richardson, and the small depths used by Elder may cause some question as to the applicability of their results to the present study.

It should also be noted that the common procedure for determining the eddy diffusion coefficient in the ocean was developed by Munk et. al. (13) and is given by:

$$k = \frac{\sigma_2^2 - \sigma_1^2}{2(t_2 - t_1)} \tag{15}$$

where k is the horizontal coefficient of eddy diffusivity, and σ_1 and σ_2 are the values of the standard deviation of the tracer concentration along a line perpendicular to the flow at t_1 and t_2, respectively.

The measured widths may be assumed to contain about 95% of the tracer thus allowing the assumption that the measured width, W, equals 4σ. Then:

$$k = \frac{W_2^2 - W_1^2}{32(t_2 - t_1)} \tag{16}$$

Also, the scale of the mixing process is assumed to be:

$$L = \frac{W_1 + W_2}{2} \tag{17}$$

(5) Field Scale Determination of the Longitudinal Mixing Coefficient

Several notable efforts have been expended towards the determination and analysis of the longitudinal mixing coefficient in rivers; however, the resulting data from these studies and subsequent analysis were restricted because of the uncontrollable flow conditions and/or non-steady state flow regime encountered.

Thomas (14) conducted experiments in the Chicago Sanitary and Ship Canal using a point source of Scandium 46 and Tritiated water, and proposed the following

equation describing the longitudinal dispersion:

$$D_L = \frac{h\,\bar{u}^3}{u_*^2}\,\phi(n) + \frac{h\,u_*^2}{\bar{u}}\,\psi(n) \qquad (18)$$

where h is the depth of flow, u_* is the shear velocity, and n is the coefficient in the velocity power law which is assumed to vary from 6 to 10. Thomas gives values for the functions $\phi(n)$ and $\psi(n)$ within the stated range. Using equation 18 it was found that the mixing coefficient was about ten times less than that computed by conventional methods. Thomas proposed that the reason for the discrepancy was the wide variation in velocity over the cross section, since the dispersion coefficient is sensitive to changes in velocity distribution.

Patterson and Gloyna (15) performed longitudinal mixing tests in the Colorado River and in the Pierce Canal using Rhodamine B as a tracer material. An instantaneous tracer injection was made and a recording fluorometer detected the flow through curves. They stated that the longitudinal mixing coefficients in the Colorado River increased with distance from the injection point because of the increasing importance of transverse shear flow mixing with distance. Several transverse mixing coefficients were also measured using tracer releases at midstream. An empirical equation describing the longitudinal mixing coefficient was presented as:

$$D_L = 0.8\, e^{0.034\,\bar{u}\sqrt{A}} \qquad (19)$$

however, the data were not sufficient to establish a statistically sound basis for the relationship developed. It should also be noted that the tests were performed downstream from a peaking power operation which would create non-steady state flow conditions and thereby raise some question as to the assumptions made

in developing the mixing analysis.

An extensive series of tests and analyses were made by Glover (16) in both laboratory flumes and in rivers. Comparisons of theoretical and test data showed good agreement in the flume tests, but natural streams yielded mixing coefficients from 10 to 50 times larger than the theory predicted. Several different approaches to the development of a mathematical model describing mixing in three dimensions were developed and several lateral and longitudinal mixing coefficients were presented. Although Mr. Glover evidently obtained a large number of both lateral and longitudinal mixing coefficients under differing flow conditions and geometries, only selected data were presented. It would be most instructive to utilize this pedantically collected information in order that comparison with other flow geometries might be established and various calculation methods be compared.

A study by Kisiel (17) in the Upper Ohio River, using Rhodamine B and a recording fluorometer demonstrated several difficulties encountered when applying the mathematical model describing mixing in a laboraotry flume to a river with irregular geometry; however, the data only served to demonstrate that more comprehensive investigations of this type are needed.

The current work of Parker (18) on the Clinch River is worthy of note, even though the studies are concerned with non-steady state and non-uniform flow conditions. These investigations serve to illustrate the usefulness of the tracer technique described herein to unusual hydraulic studies.

An excellent review of existing knowledge from dye dispersion studies by Diachisin (19) should be mentioned. This paper developed the mathematical models for one, two and three dimensional diffusion, reviewed the methodology for the determination of mixing coefficients, and presented some field data on diffusion coefficients.

Perusal of the literature has demonstrated that although several investigations have yielded information on a particular river under an existing flow condition the data necessary to predict and understand the diffusion phenomenon are not available. It is obvious that in order to more fully delineate the parameters involved in the overall mixing process in inland waterways, controlled data from field scale measurements are required.

b. Reaeration:

(1) Basic Mechanism of Oxygen Absorption:

Probably the most important aspect of all waste water disposal problems faced by the sanitary engineer is the ultimate disposition of the effluent from a waste treatment process stream. Waste waters must eventually find their way into some phase of the hydrologic cycle, thereby contributing contamination or pollution, or both, to an essential part of the environment. Decomposition of an organic waste discharge into a body of water causes a depletion of the waters oxygen resources. Oxygen thus removed from the water can normally be replaced through atmospheric aeration, but if aeration is insufficient to maintain an adequate oxygen concentration, conditions in the receiving water may become intolerable for aquatic life.

It is generally agreed that the ability of a body of water to assimilate organic waste is dependent on the oxygen absorption characteristics of the water, and that a practical method of determining oxygen absorption rates would greatly aid the design engineer in determining the degree of treatment required for a proposed waste discharge.

Although the controlling mechanism of the gas transfer process must be related to molecular motion, sustained absorption of a gas into a liquid must be accomplished by some mechanism related to turbulence intensity. It is this mechanism that has

been the subject of study in attempts to establish a relationship between reaeration and stream hydrodynamics. The fundamental concepts of gas absorption developed prior to 1960 have been pedantically discussed in a paper by Krenkel and Orlob (20) and will not be elucidated here.

Recent notable investigations into the reaeration phenomenon include the work of Churchill et. al. (21) where exhaustive statistical analysis of oxygen uptake rates and river hydraulic characteristics resulted in the following empirical equation:

$$k_2 = 5.026\ \bar{u}^{0.969}\ R^{-1.673} \qquad (20)$$

where k_2 is the reaeration coefficient in days^{-1}, $\bar{u}$ is the mean stream velocity, and R is the mean stream depth. Although this relationship appears to be valid for the particular streams from which derived, one could easily visualize different flow geometries that would yield erroneous results and yet have the same velocity and depth. Churchill used many parameters in his correlation analyses; however, even though no theoretical basis for equation 20 exists, and the correlation for this particular equation was no greater than any other, it was stated to be the most useful. It is apparent that a relationship will exist between the parameters included in equation 20 if the velocity is taken as a measure of turbulence intensity and the depth is assumed to be related to the mixing length; however, it is believed that the relationship will be valid only for the streams from which derived, as indicated by Streeter (22).

It should be noted that the data collected by Mr. Churchill is probably the only extensive source of true oxygen uptake rates for rivers available in the literature. These measurements were taken below an impoundment where the water released approached zero in dissolved oxygen content because of its withdrawl from

the hypolimnion, and where the discharges were controlled and predictable. It should be noted that this arrangement makes the sites utilized by Churchill ideal for the investigations described herein.

Dobbins (23) investigated the mathematical model describing gas absorption using Hydrogen, Oxygen, Nitrogen, Propane and Helium introduced into a covered kettle in which varying mixing regimes could be produced. He found that the absorption coefficient was dependent on the molecular diffusivity, which is contradictory to the results found by Kishinevski (24), (25), who reached the conclusion that the assumption of a laminar surface film is erroneous and that the absorption process is controlled in most instances by turbulent diffusion. It would be most informative to determine which investigator is in error, as Kishinevski also presented experimental evidence to substantiate his assumption that absorption coefficients were the same for all gases undergoing identical mixing.

In another paper, Dobbins (26) extended and modified the Streeter-Phelps equation to include various sources of oxygen supply and demand which were not included in the original formulation. He also mathematically investigated the effects of the longitudinal mixing coefficient on the BOD and oxygen profiles in fresh water streams and concluded that its effect was negligible. It should be noted, however, that although the longitudinal mixing coefficient may not play a significant role in a mass balance such as described by Dobbins, it is directly related to oxygen gas transfer in a river, because it is a direct measure of turbulence intensity, and is treated as such in these studies.

Dobbins utilized a previously formulated mathematical model describing gas absorption (27) which is:

$$k_L = \sqrt{D_m r}\, \coth \sqrt{\frac{rL^2}{D_m}} \qquad (21)$$

where D_m is the molecular diffusion coefficient of the gas, r is the average surface renewal rate, and L is the liquid film thickness. The analysis presented by Dobbins was checked using data from both field and laboratory measurements of reaeration and the results appear to give much credulence to the Film Replacement Theory and its modifications as proposed by Dobbins. Because of its potential usefulness in these studies, the comparison of computed and reported values of k_2 presented by Dobbins is shown on Figure 1.

Other studies performed during the past few years on stream reaeration not pertinent to this study, but worthy of mention, include a paper by O'Connor (29) who attempted to eliminate the time of flow as an unknown in Streeter's Equation and indicated the effect of flow on the stream coefficients and on pollution capacity; and additional studies by the British (30), (31) who utilized their methodology for assimilation capacity which involves the introduction of sodium sulfite into the river and subsequent measurement of oxygen uptake rates.

It should be noted that although these previously described investigations have all added to the status of knowledge of stream reaeration, what is truly needed is not more theory, but additional field measurements of oxygen uptake rates such that the proposed mathematical models can be verified or discarded. There is still a pressing need for a method by which the regulatory agency or consulting engineer can intelligently predict the waste assimilation capacity of a receiving water.

c. Pulse Testing Techniques:

Time domain solutions of the differential equations describing turbulent mixing phenomena are most difficult to obtain even in the case of a simple physical situation. Solutions are usually found for idealized boundary conditions such as an instantaneous injection. In many cases, it is relatively simple

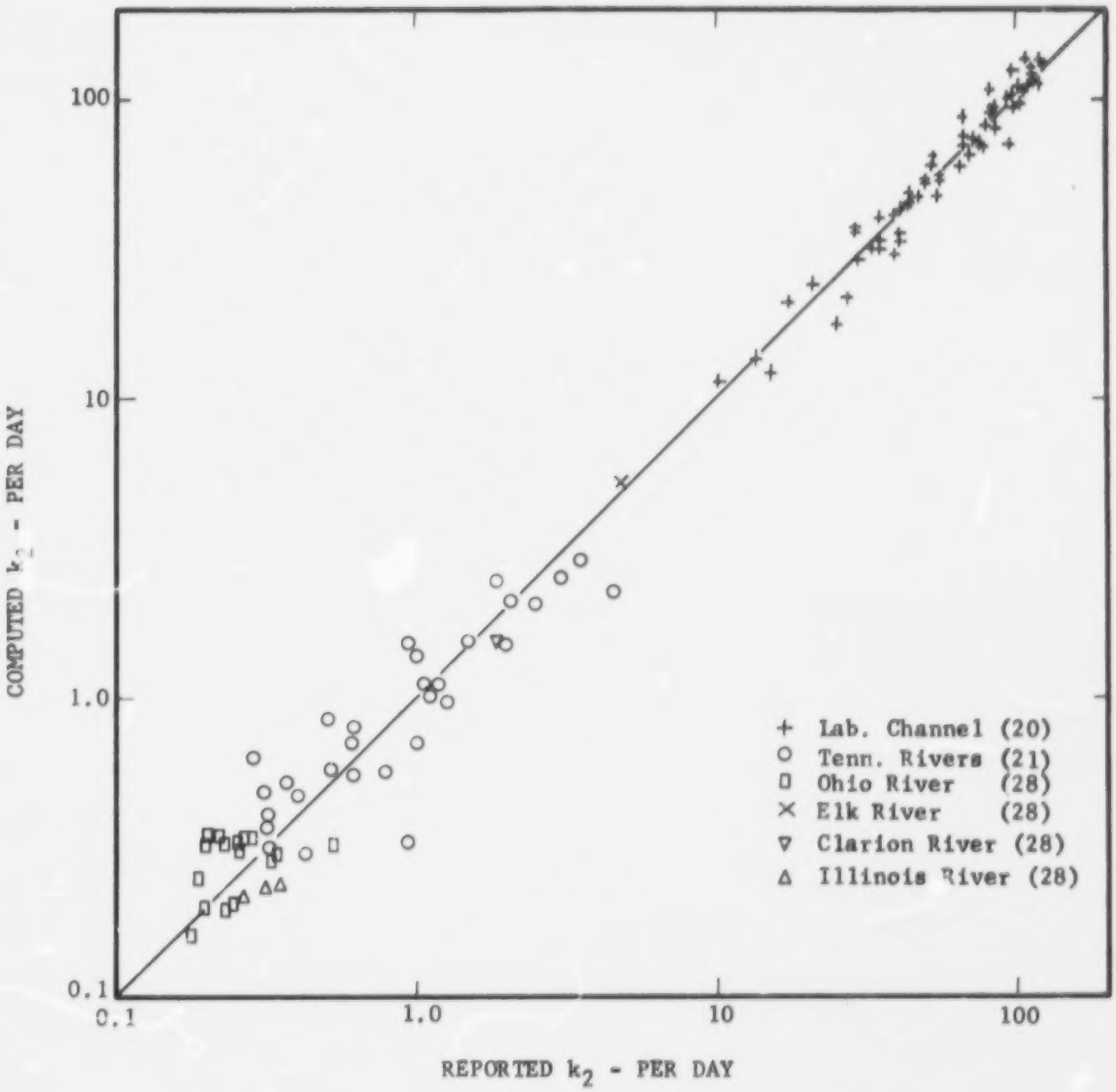

FIGURE I: COMPARISON OF COMPUTED & REPORTED k_2
(after Dobbins)

to find frequency domain solutions to the same differential equations. Thus an experimental method that efficiently produces frequency response information is a highly desirable research implement. There are two commonly employed methods for obtaining frequency response, direct sinusoidal testing and pulse testing. The advantages and disadvantages of both methods have been reviewed by Clements (32) in his doctoral thesis. Perhaps the greatest advantages of the pulse method are in its potential economy of testing time, the short loss of production time of applying the method to a manufacturing or processing plant, and the ease with which a pulse in the independent variable may be made.

The first practical use of pulse testing appears to have been in obtaining the frequency response of aircraft for use in the designing of control servos for autopilot mechanisms. Smith and Triplett (33) have presented a review of this method as applied to aircraft, and discussed the effect of the frequency content of the input pulse and the effect of pulse shape on this frequency content. They first explained certain practical limitations inherent to the mathematical derivations and in the treatment of experimental data. Further investigations into these topics are given by Hougen and Walsh (34), Dreifke (35), and Dreifke, Hougen, and Mesmer (36). Clements and Schnelle (37) reported on further extensions of the theory and presented a rather simplified review of the subject of pulse testing.

Draper, McKay, and Lees (38) described in detail the general mathematical background for dynamic testing, and, the mathematical basis for numerical Fourier transforms and graphical forms of transfer functions was developed. This material is reviewed again by Lees (39) in a paper describing the general area of pulse testing and methods of dynamic measurement and data reduction.

In addition to the publications listed above there have been other applications of dynamic testing and in particular pulse testing to servo-mechanisms, control apparatus, and chemical processing equipment. Two reports from the Instrumentation Laboratory of the Massachusetts Institute of Technology (40), (41), were concerned with the pulse testing of various servo and control apparatus. Lees and Hougen (42) published the results of a study comparing pulse and sinusoidal methods in the dynamic testing of a shell and tube heat exchanger obtaining excellent agreement between the two methods. Stewart, Sliepcevich, and Puckett (43), have examined the dynamics of a stirred kettle using pulse tests, and Hougen and Walsh (34) described various other applications in problems of chemical engineering interest. Also, an excellent summary of current research work in dynamic testing is given in the A.I.Ch.E. Symposium Series (#36, Process Dynaimcs and Control and #46, Process Systems Engineering).

This list is not an exhaustive compilation of references pertinent to pulse testing. It is believed that sufficient information is given such that an understanding of the potential of this method can be obtained by perusal of the literature quoted.

II ACCOMPLISHMENTS MADE DURING REPORT PERIOD

1. Construction of Model

As described in the initial proposal for this research investigation, the first year's effort was expended towards the design and construction of a suitable laboratory flume in which the studies described herein could be pursued. The resulting structure has proven to be ideal for these studies and although several modifications must be made, the dispersion studies planned for the summer of 1964 are presently underway.

The flume is 60 feet long, 2 feet wide and one foot deep and is supported at the third points by a knife edge and a worm gear such that the slope may easily be varied. The open channel section is glass walled so that measurement techniques are facilitated and side wall effects are minimized. A constant speed propeller pump driven by a variable speed D.C. motor recirculates the flow through two stainless steel return pipes which can be operated singly or together by means of a diversion gate. Artificial roughness in the channel is created by the use of expanded screen mesh laid on the flume bottom and an egg crate type baffle is used at the inlet to minimize entrance effects. The depth is measured by use of a travelling point gage that rides on two rails extending the length of the flume and also travels on a rail transverse to the flume such that variations in the bottom can be determined.

Flow measurement is presently being accomplished utilizing tracer techniques; however, it is planned to insert an orifice meter in each return pipe at the earliest opportunity. Figures two through seven show pertinent details of the structure as previously described.

2. Analysis of Tracer Methodology

a. Surface Diffusivity:

In order to measure the surface diffusivity, the method of Orlob has been adapted for use in the experimental flume. One-sixteenth inch diameter polyethelene particles are released, each in an identical manner, to simulate a point source. The particles are then collected at known distances downstream in a multi-celled screened collector, such that a distribution analysis can be made. A picture of the particle collecter is shown on Figure 9 and a typical set of data is shown on Figure 8. The analysis has been performed at various locations transverse to the flume to insure homogeneity and the results indicate that this

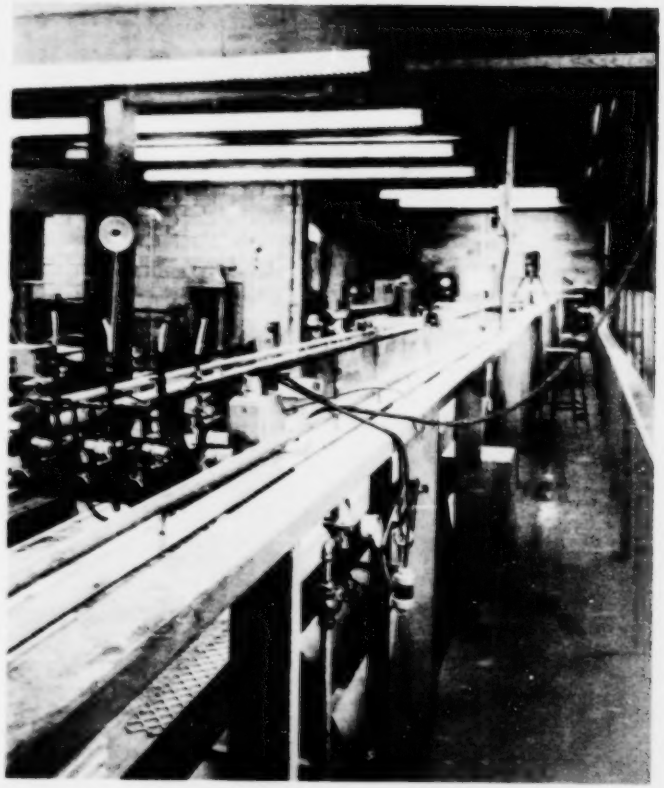

FIGURE 2: GENERAL VIEW OF FLUME SHOWING PULSING PUMPS

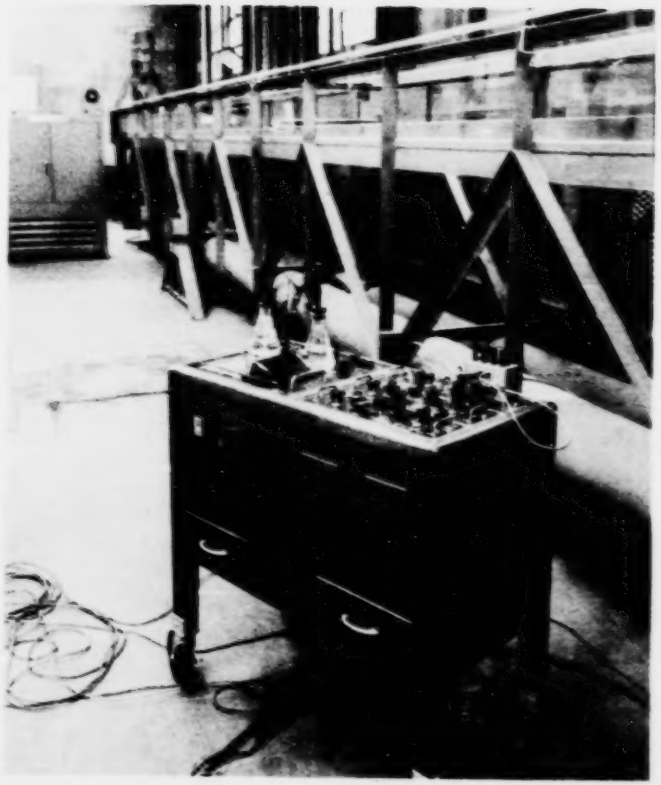

FIGURE 3: SANBORN RECORDER

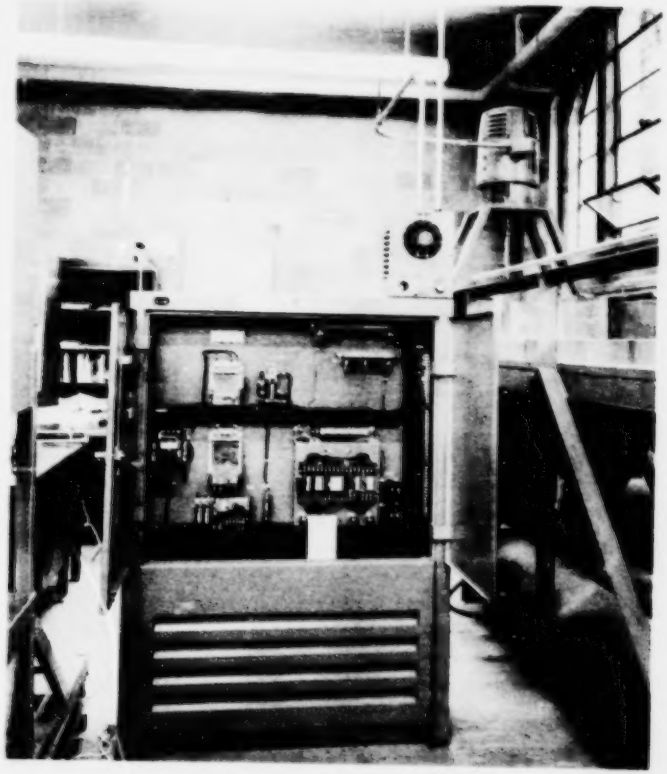

FIGURE 4: D.C. SPEED VARIATOR

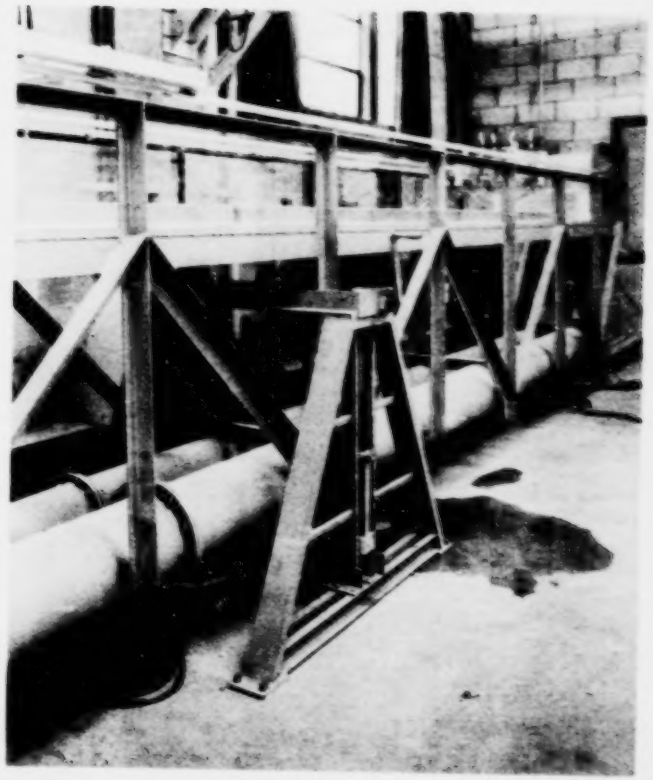

FIGURE 5: WORM GEAR FOR SLOPE ADJUSTMENT

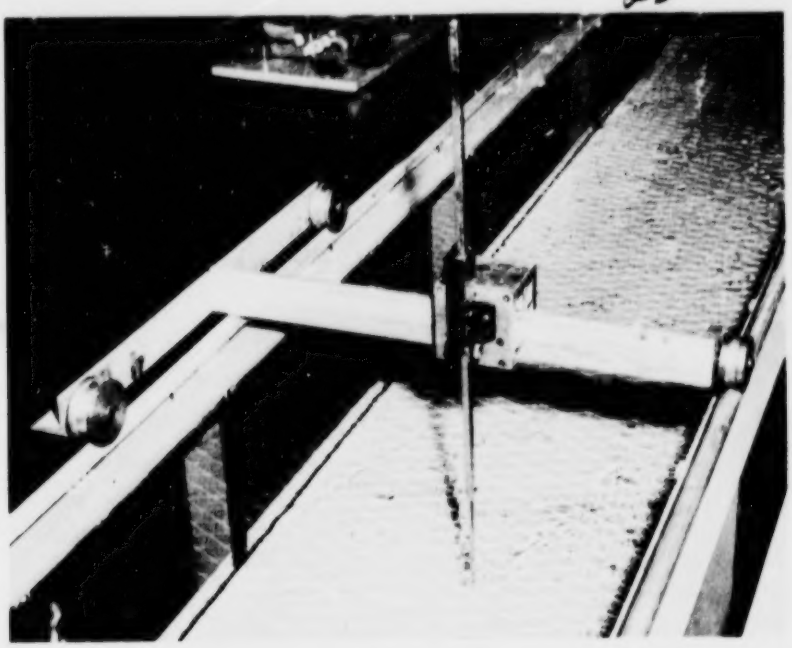

FIGURE 6: TRAVELING POINT GAGE

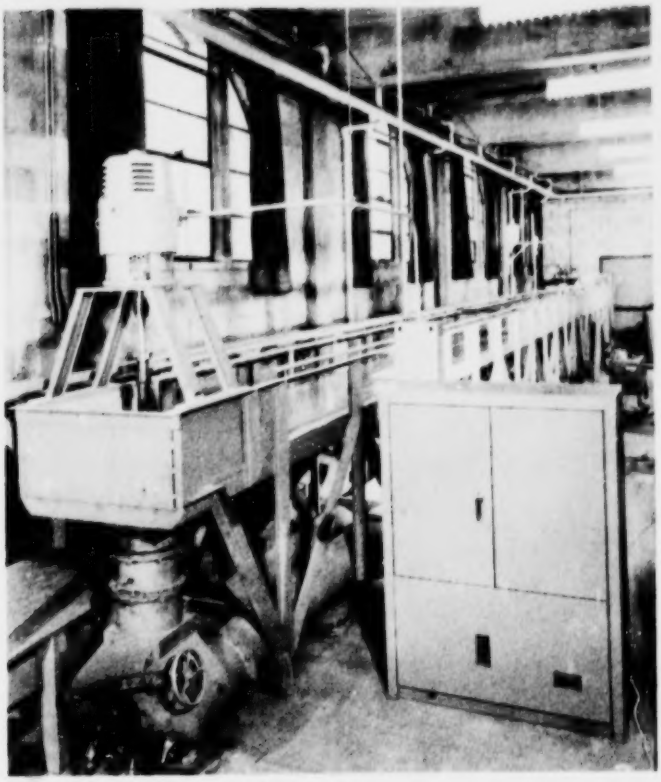

FIGURE 7: RECIRCULATING PUMP AND CONTROL VALVE

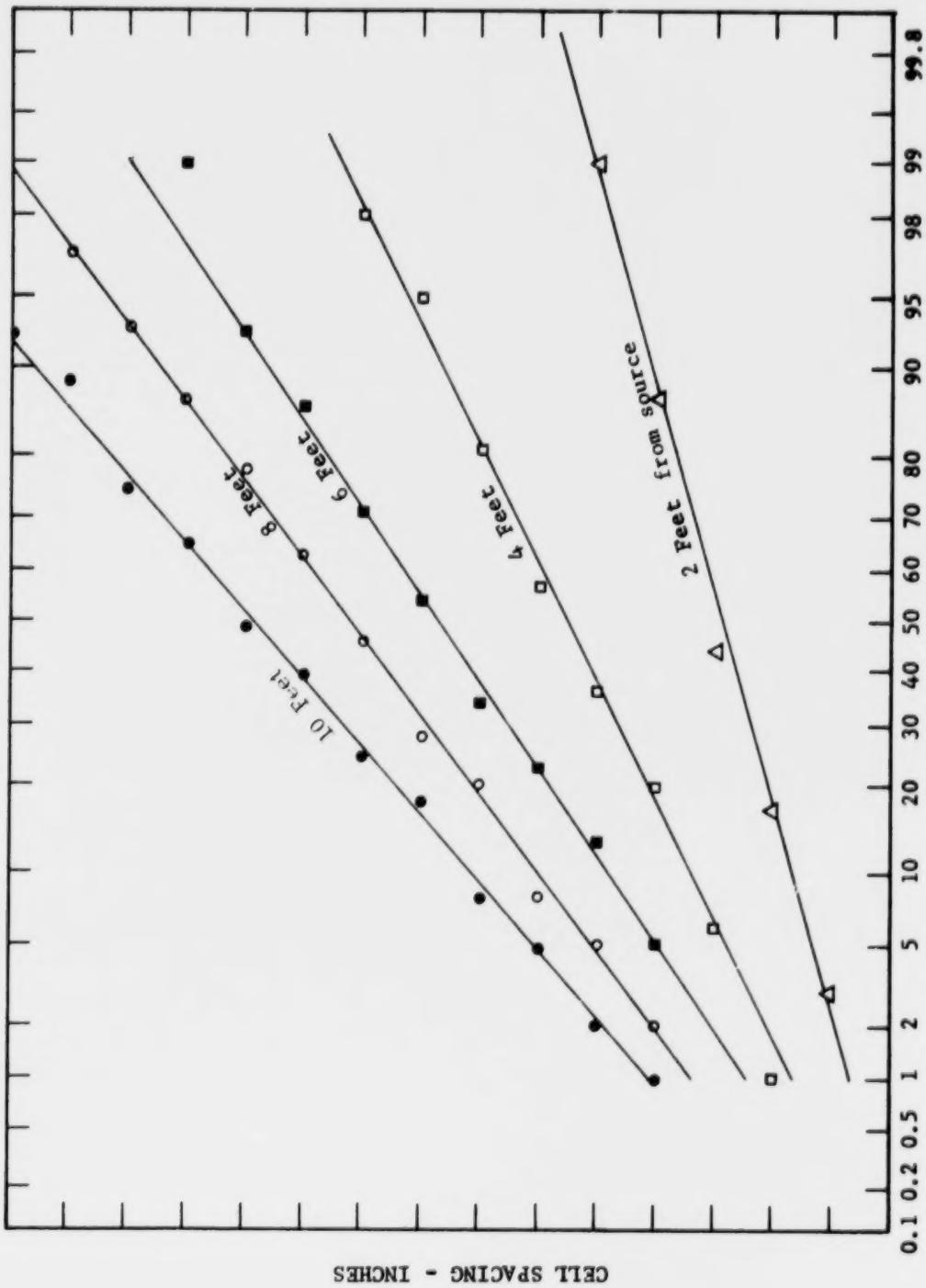
CELL SPACING - INCHES
0.1 0.2 0.5 1 2 5 10 20 30 40 50 60 70 80 90 95 98 99 99.8
ACCUMULATED PARTICLES - PER CENT OF TOTAL
2 Feet from source
4 Feet
6 Feet
8 Feet
10 Feet

FIGURE 8: TYPICAL DISTRIBUTION OF PARTICLES RELEASED FROM POINT SOURCE

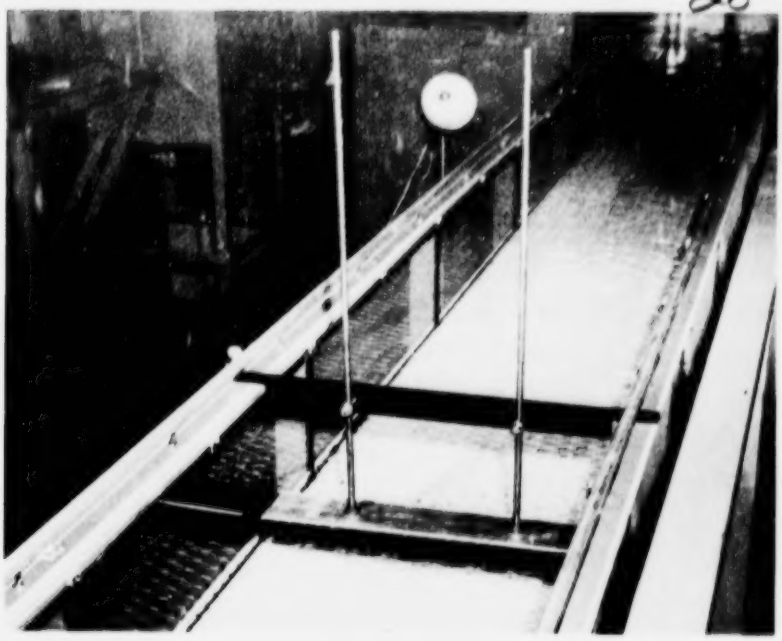

FIGURE 9: PARTICLE COLLECTOR

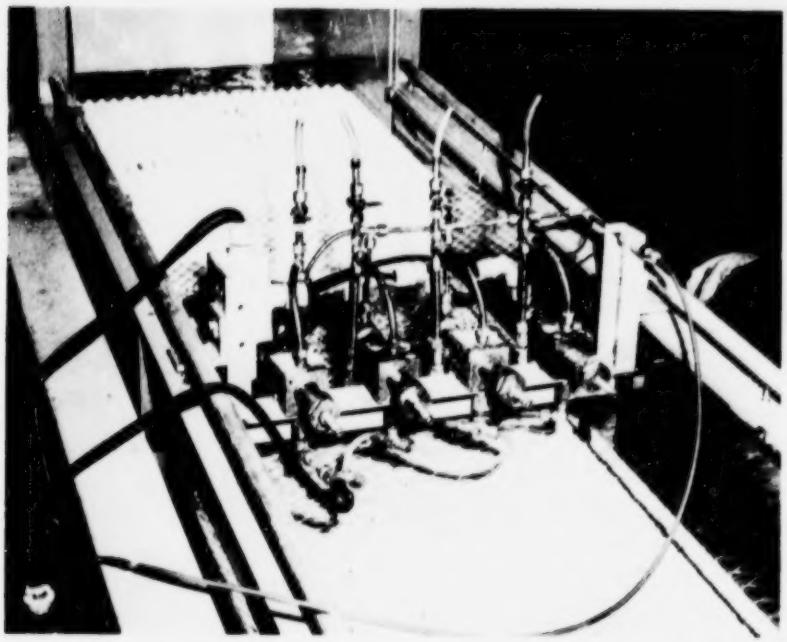

FIGURE 10: PULSING PUMPS

turbulence measurement scheme is adequate. The standard deviation is determined from the statistical analysis of particle distribution and the surface diffusion coefficient is determined utilizing equation 14. It should be noted that the mixing length can also be determined using a method devised by Orlob.

The surface diffusivity, as measured in these tests, is identical to the diffusivity measured by engineers in the designs of ocean outfalls and as described in a previous section of this report. Measurement of this parameter is now routine and it is expected that a most useful array of surface diffusivities under widely varying hydraulic conditions will be available by the end of this summers efforts.

It is also planned to determine this parameter in the field studies to be conducted in the latter part of the summer of 1964; however, the methodology that will be utilized has not yet been refined. Preliminary tests indicate that the major difficulty encountered will be in the collection of tracer particles such that a statistical analysis of their distribution may be determined.

b. Lateral and Vertical Diffusivity:

The lateral and vertical diffusivities will be measured using a point source of tracer material injected into the flowing stream by means of a small diameter jet. Since the introduction of tracer must be at the same velocity of the stream, a continuous type infusion pump is used to allow a constant metered quantity of tracer to be introduced for a sustained period of time. When steady state conditions have been reached, samples of the tracer plume are taken at intervals transverse to the stream for the horizontal diffusion coefficient, and vertical to the stream for the vertical diffusion coefficient. If this procedure is pursued at various known distances downstream from the diffuser, the diffusion coefficients can be determined by utilizing the analysis described by Pien.

The tracer distribution at any given point in the jet stream will very closely describe a normal error curve. Thus, the standard deviation may be obtained via statistical analysis and the appropriate diffusion coefficient may be computed utilizing the Einstein equation. Both fluorescent dye and conductive material have been used for this determination and corresponding analysis by fluorometric and conductimetric techniques have been used.

The river survey planned for the summer of 1964 will include measurements of these parameters in a flowing stream. A portable pump will supply a constant feed of dye to be injected as a continuous point source through a nozzle held in position by floats. This procedure has been used by Parker and has been found satisfactory. A 12 volt portable pump will be used to sample the tracer plume at predetermined distances in order that the tracer distribution can be determined and the diffusion coefficient computed. The inlet to the pump is supplied with a 50 foot hose weighted by a Price Current Meter Bomb, and samples can be collected in about 30 seconds including flushing time.

Since the physical characteristics of the hydraulic system to be used are known, the vertical diffusion coefficient may also be computed utilizing the formulation

$$\bar{\epsilon}_y = \frac{\kappa}{6} h u_* = \frac{\kappa}{6} h \sqrt{\frac{\tau_o}{\rho}} = \frac{\kappa}{6} h \sqrt{ghS} \qquad (22)$$

where $\bar{\epsilon}_y$ is the average vertical eddy diffusivity, κ is von Karmans constant taken as 0.4, u_* denotes the shear velocity, τ_o is the boundary shear stress, ρ is the density of water, g represents the gravitational constant, and S is the slope of the energy gradient.

It will be instructive to note the correlation between this approach to the calculation of vertical diffusion coefficients and the measured values obtained

in the experimental flume. Churchill computed this parameter utilizing equation 22 in his reaeration studies in the TVA area and attempted to correlate the computed values with the reaeration coefficient. He was apparently unsuccessful in establishing this relationship even though the gas transfer process should be directly related to the vertical diffusivity if it is a true measure of surface renewal.

c. Longitudinal Mixing Coefficient:

The longitudinal mixing coefficient is determined by sudden injection of the tracer material into the flume and subsequent measurement of the time concentration curve at downstream stations. The tracer material, which is a sodium chloride solution is injected as a line source by means of four pulsing pumps, shown on Figure 10, which are actuated under pressure by solenoids and yield an essentially instantaneous line source of tracer material.

The flow through curve is detected by means of platinized conductivity probes located at two stations downstream and forming the fourth leg of a Wheatstone Bridge circuit. The concentration changes are detected and plotted on a two channel Sanborn carrier-amplifier-recorder system as a permanent record. The traces are then analyzed by previously described analytical techniques and the longitudinal mixing coefficient and mean stream velocity are determined. This system is described in detail in a paper by Krenkel (44).

The longitudinal mixing coefficient will be determined in the field surveys by using an instantaneous dose of Rhodamine B injected into the river, and following the tracer flow-through curve at several stations downstream. Because of inherent difficulties with automatic recording systems, grab samples will be taken for subsequent analysis even though continuous fluorometric recorders will be used.

d. Correlation of Experimental Results:

Obviously, in any given turbulent flow system, the mixing parameters described in the preceeding discussion must be related. There is much confusion existing in the literature both as to definitions of these diffusion coefficients and as to what they indicate in terms of water quality studies (45). The results of these experiments will show the desired interrelationships and furthermore, should establish a criterion for defining mixing coefficients in water quality studies.

The results of the flume investigations will be analyzed both theoretically and statistically using a digital computer. Also, it is expected that the field data collected will reveal much needed information, even though there will not be as many observations as can be made in the laboratory flume.

It should be noted that the reaeration coefficients in the streams to be used have already been pedantically determined by Churchill, and thus hopefully, the question of mixing coefficients and their relation to reaeration should be resolved. Also, since the stream sections to be utilized are immediately below impoundments, these investigations can be carried out under given steady-state flow conditions by previous arrangement with the regulatory agencies involved.

3. Application of Mathematical Model to Observed Data

During the summer of 1963, 26 separate runs were made on the flume with at least two determinations of the dispersion coefficient being made on each run. In all, 59 usable flow-through traces were obtained. The conditions of each run were chosen to produce a wide range of energy slopes, water depths, and average velocities. The dispersion coefficients were calculated using Levenspiel's statistical method which has been previously described.

The average flow-through time was chosen as the time from injection of the

salt tracer to the peak of the time-concentration curve and the length of channel between injection and measurement was divided by this value of time to obtain $\bar{u}$, the average velocity. In about 90 percent of the trials, the predicted curve appeared prematurely on the time scale, peaked too quickly, and disappeared too soon. However, the shape of the predicted curve and the value of the predicted peak concentration were essentially the same as the observed curve. This early appearance phenomenon, which was caused by using a value of average velocity which was too high, indicated that the modal value of the time-concentration curve does not really represent the average flow-through time, as was previously shown.

Levenspiel's theoretical expression for the average flow-through time indicates that it is always greater than the modal value of the concentration by a time dependent on $D_L/\bar{u}L$. The greater the influence of turbulent dispersion relative to convective transport, the more the tracer cloud will diffuse as it passes the point of measurement, the more skewed the time-concentration curve will be, and the more the average flow-through time will differ from the time to the modal value of concentration. Levenspiel states that if $D_L/\bar{u}L$ becomes as large as 0.01, the average flow-through time will be significantly greater than the time to the peak concentration value.

With this in mind, values of $D_L/\bar{u}L$ were calculated for each dispersion coefficient determination. They ranged from about 0.004 to 0.021, the majority being between 0.01 and 0.015. This indicated that the assumed values of average flow-through time which were used in calculating the dispersion coefficients were indeed too low and were the cause of the early appearance and die-away of the predicted curve relative to the observed curve.

Since flow in the channel was not metered, the average velocity and average

flow-through time could not be determined directly. Thus, the observed time difference between the observed and predicted curves was added to the originally used time to peak to produce another estimate of average flow-through time. This was used to re-compute the average velocity and the dispersion coefficient. A second predicted flow-through curve was then calculated and plotted on the strip chart with the observed curve. These curves matched in the time scale in every case except for the extreme tails of curves where it is doubtful that the mathematical model used in computing the distributions was valid.

It was found that values of the dispersion coefficient which were too high or too low, giving predicted peak concentrations which were too low or too high respectively, could be corrected without recalculation by multiplying the coefficient used by the square of the ratio of the calculated to the observed peak concentration. This can be done only if the time to peak differential has been eliminated first and if the observed and predicted peak concentrations occur at essentially the same time.

This simple correction is possible because, at peak concentration, dC/dt is zero and the exponential term in equation (2) becomes unity, leaving

$$C = \frac{M}{2A\sqrt{\pi D_L t}} \tag{23}$$

Here it can be seen that the ratio of two dispersion coefficients would depend only on the ratio of the squares of concentration as long as time is the same in both cases.

Experimenting with methods of predicting the average flow-through time without such a long trial-and-error process resulted in the observation that a value of time very close to that determined by trial-and-error can be obtained

by using the midpoint of a line connecting the two points of inflection of the curve. Future mathematical analysis will determine if this empirical method has any basis in theory and if it can be used with success on curves from other sources with values of $D_L/\bar{u}L$ different from the ones produced in this flume.

In general, the observed flow-through curves fit the mathematical model for dispersion (equation 3) very well, with the exception of the tails. The leading tail and the first part of the rising leg of the observed curve were always lower than predicted. This was balanced by a lagging tail which was almost always higher than predicted and the middle portion of the curve and the falling leg were essentially the same as predicted. The discrepancy was believed to be caused by part of the tracer initially being trapped in the expanded wire mesh on the bottom used to produce turbulence and not reaching the measurement point until after the main cloud of tracer had passed, when it was slowly released into the then tracer-free overflowing water to produce the extra-long lagging tail which was observed.

It was found that flow-through curves with extra long lagging tails gave a calculated dispersion coefficient which was too high; and curves which lacked any leading tail, but started abruptly and rose steeply, gave a calculated coefficient which was too low. A typical analysis of a flow through curve and its modifications is shown on Figure 11.

4. Pulse Testing Techniques

The theory, development, and application of the pulse testing technique to water quality studies as performed during the grant period has been presented at the 1964 Purdue Industrial Wastes Conference and is included as an appendix to this report.

Perusal of this material will demonstrate the potential of frequency response methodology to the sanitary and water resources engineering field, and the progress

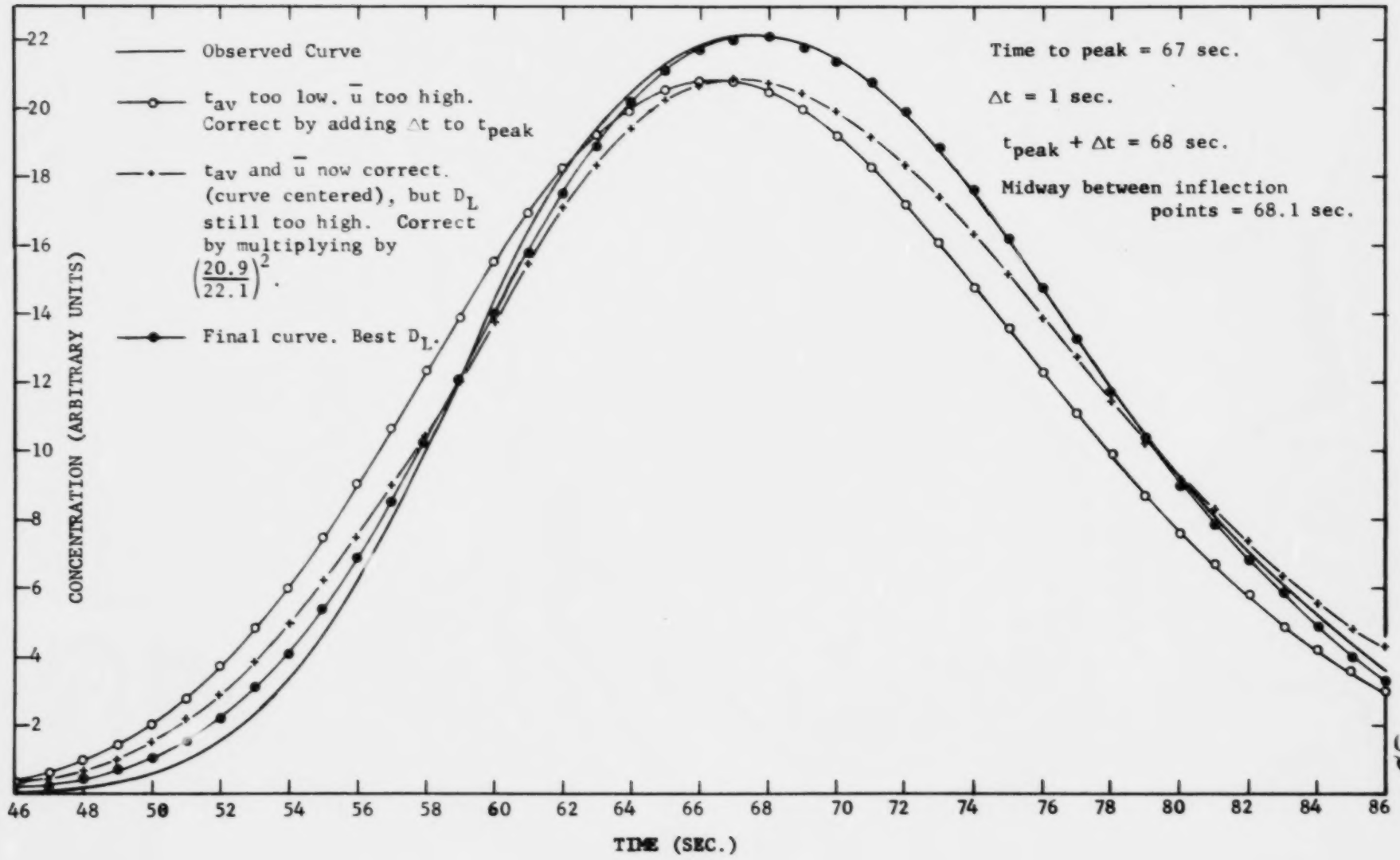

FIGURE 11: TYPICAL TIME-CONCENTRATION CURVE ANALYSIS

and accomplishments demonstrated certainly justify inclusion of the chemical engineering profession in this research.

5. Reaeration and Longitudinal Dispersion

Previous investigations have demonstrated a relationship between the longitudinal mixing coefficient and the reaeration coefficient (20) as given by the equation:

$$k_2 = (\text{constant})\, e^{\frac{-E_a}{RT}} D_L h^{-2} \qquad (24)$$

where $e^{\frac{-E_a}{RT}}$ is the probability of the activated state, E_a is the activation energy, R is the universal gas constant and T is the temperature. From Kolmogoroff's Similarity principle, it follows that a similar relationship should be obtained if energy expenditure per unit mass of fluid is related to the reaeration coefficient and a measure of scale. Krenkel (20) demonstrated this relationship in a laboratory flume and found that:

$$k_2 = 1.14 \times 10^{-4} E^{0.408} h^{-0.660} \qquad (25)$$

Since the correlation coefficient of 0.86 indicates that this relationship has considerable merit, the results of Churchill's measurements (21) were plotted in a similar manner as shown on Figure 12 with the dimensionally correct exponents of $E^{1/3}$ and $h^{-2/3}$. The resulting line of best fit of Churchill's data, which are accurate reaeration measurements on rivers, was described by:

$$k_2 = 0.89 \times 10^{-4} E^{1/3} h^{-2/3} \qquad (26)$$

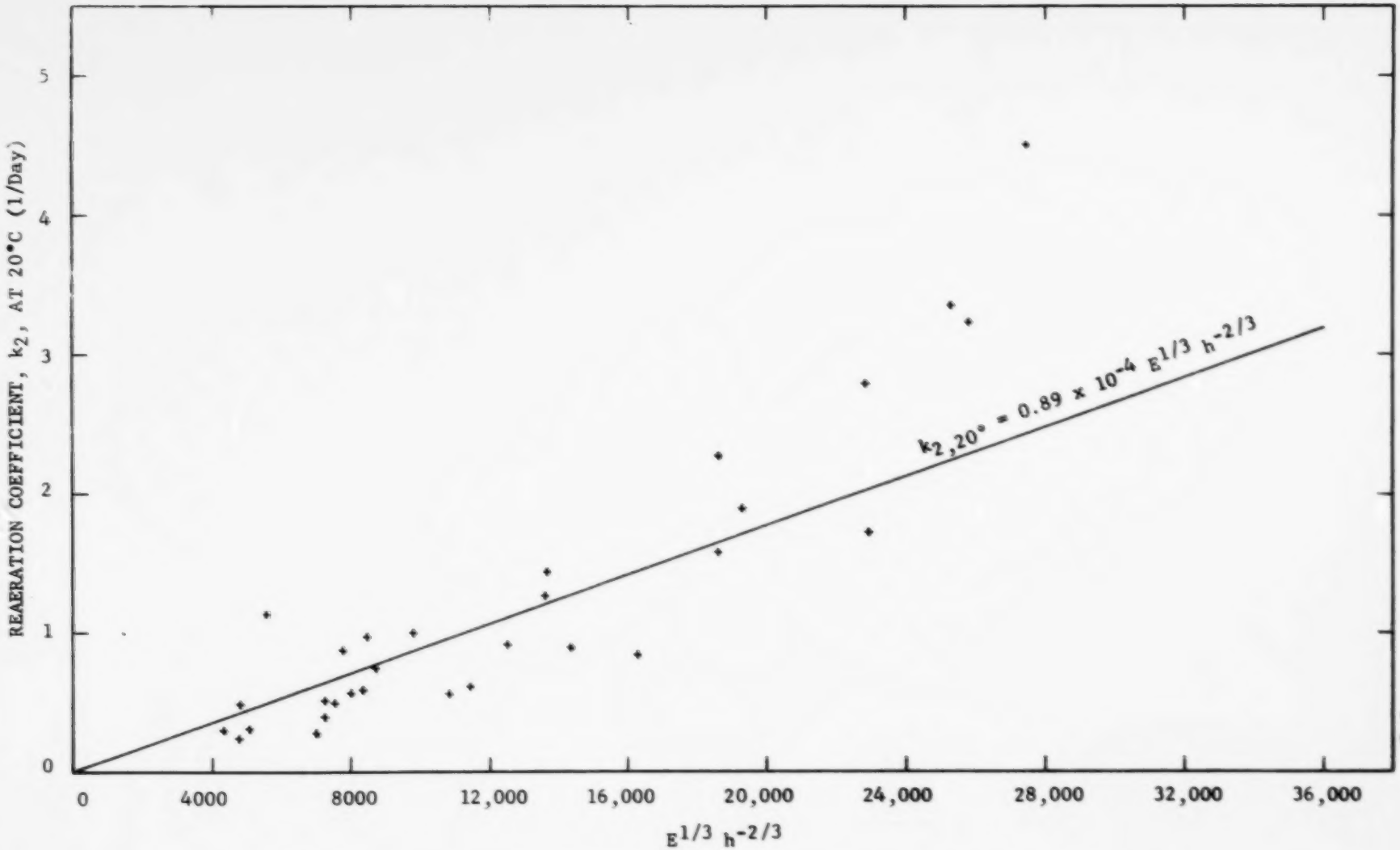

FIGURE 12: ENERGY EXPENDITURE AND THE REAERATION COEFFICIENT

The similarity of these equations is remarkable, considering the fact that equation 25 was obtained from a one foot laboratory flume and equation 26 was obtained from rivers up to 700 feet in width. For this reason, continued effort will be expended in the theoretical aspects of the proposed relationships and additional reaeration measurements will be made in the laboratory flume and in the river, if time permits.

The relation of energy expenditure to gas absorption is entirely reasonable and would also be a most desirable approach to aeration studies in bounded vessels if a method of measuring a vessel mixing length parameter were available. The advantages of this measurement technique for stream reaeration studies are obvious, for presumably, the only measurements required would be the stream velocity, the slope of the energy gradient and the depth, which is assumed to be a measure of scale.

6. The Longitudinal Mixing Coefficient & Energy Expenditure

The difficulties encountered in the field scale determination of the longitudinal mixing coefficient immediately demonstrates the desirability of investigating new measurement techniques. The heuristic thought occurs at once that perhaps the Kolmogoroff principle (46), which predicts a relationship between the mixing coefficient, the energy expenditure, and a measure of scale, could be conveniently utilized. Perhaps it may be feasible that the mixing properties of tidal estuaries could be obtained using this concept, estimating the energy dissipation from formulations such as those proposed by Taylor (47).

Experiments conducted both at California and Vanderbilt have demonstrated conclusively that the energy expenditure can be related to the mixing coefficient if the depth of flow is taken as a measure of scale in a laboratory flume.

The energy expenditure per unit mass of fluid per unit time, E, was defined

as:

$$E = \bar{u} S_e g \tag{27}$$

where $\bar{u}$ is the mean stream velocity, S_e is the slope of the energy gradient and g is the gravitational constant.

If the basic formulation of Kolmogoroff is utilized, the functional relationship should appear as:

$$D_L = \text{Constant } h^{4/3} E^{1/3} \tag{28}$$

where h is a measure of the scale, which in these experiments was assumed to be related to the depth of flow.

In order to test the validity of this relationship, a series of experiments were conducted on a one foot wide flume, using expanded metal mesh as the bottom roughness. The results of these experiments are shown on figure 13 and yielded the following regression equation:

$$D_L = 6.425\, E^{0.296}\, h^{1.243} \tag{29}$$

The correlation coefficient of this analysis was 0.99 which indicates an unusually high correlation for data of this type.

Another series of data were taken on a 2 foot wide glass walled flume and are shown plotted with the previously obtained relationship. These data indicate the same functional relationship between the variables but with a slightly different constant. If the apparent constant is assumed to be a function of roughness, as suggested by Ichiye (48), the universality of the proposed relation could be established. Investigations are presently being conducted to

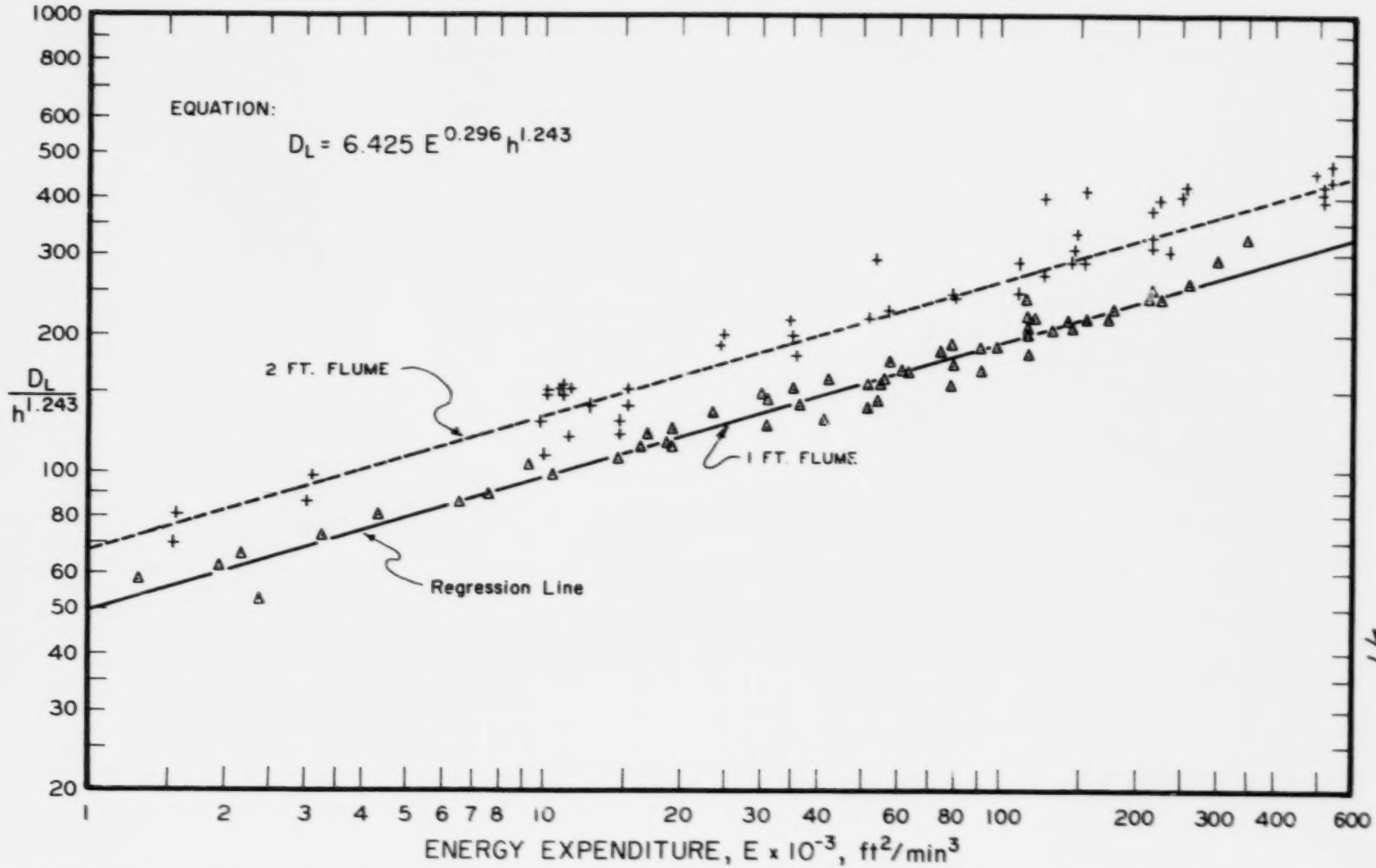

FIGURE 13: RELATION BETWEEN THE MIXING COEFFICIENT AND THE ENERGY DISSIPATION

determine the nature and effect of this "constant" in the flume at Vanderbilt University.

It is interesting to note that a similar relationship was derived from data taken from Orlob's (9) investigations on a four foot wide flume. Again utilizing the depth as a measure of scale and equation 23, the following regression equation resulted and is shown on Figure 14:

$$D_z(10^3) = 96.1\ E^{0.504}\ h^{1.19} \tag{30}$$

where D_z is the lateral surface diffusivity as determined by the lateral movement of polyethelene particles on the water surface. Although this equation is based on a different parameter of mixing, D_z, one would expect a similar relationship because of the interdependence of the various mixing coefficients.

Because most attempts to predict the longitudinal dispersion coefficient from known hydraulic parameters have either relied on equation 28 or

$$D_z = \text{constant}\ h\ u_* \tag{31}$$

initial investigation in the realm of correlation investigation involved plotting the calculated values of D_L against $h^{4/3}E^{1/3}$ and against hu_*. In both cases, excellent correlation was obtained and the points described a straight line with some scatter apparently due to experimental error. In each case the slope of the line was greater than that obtained from a similar plot of values obtained by Krenkel from a flume at the University of California, the difference being in the range of 20 to 30 per cent. A reduction of the difference to the range of 10 to 20 per cent was achieved by using the distance from

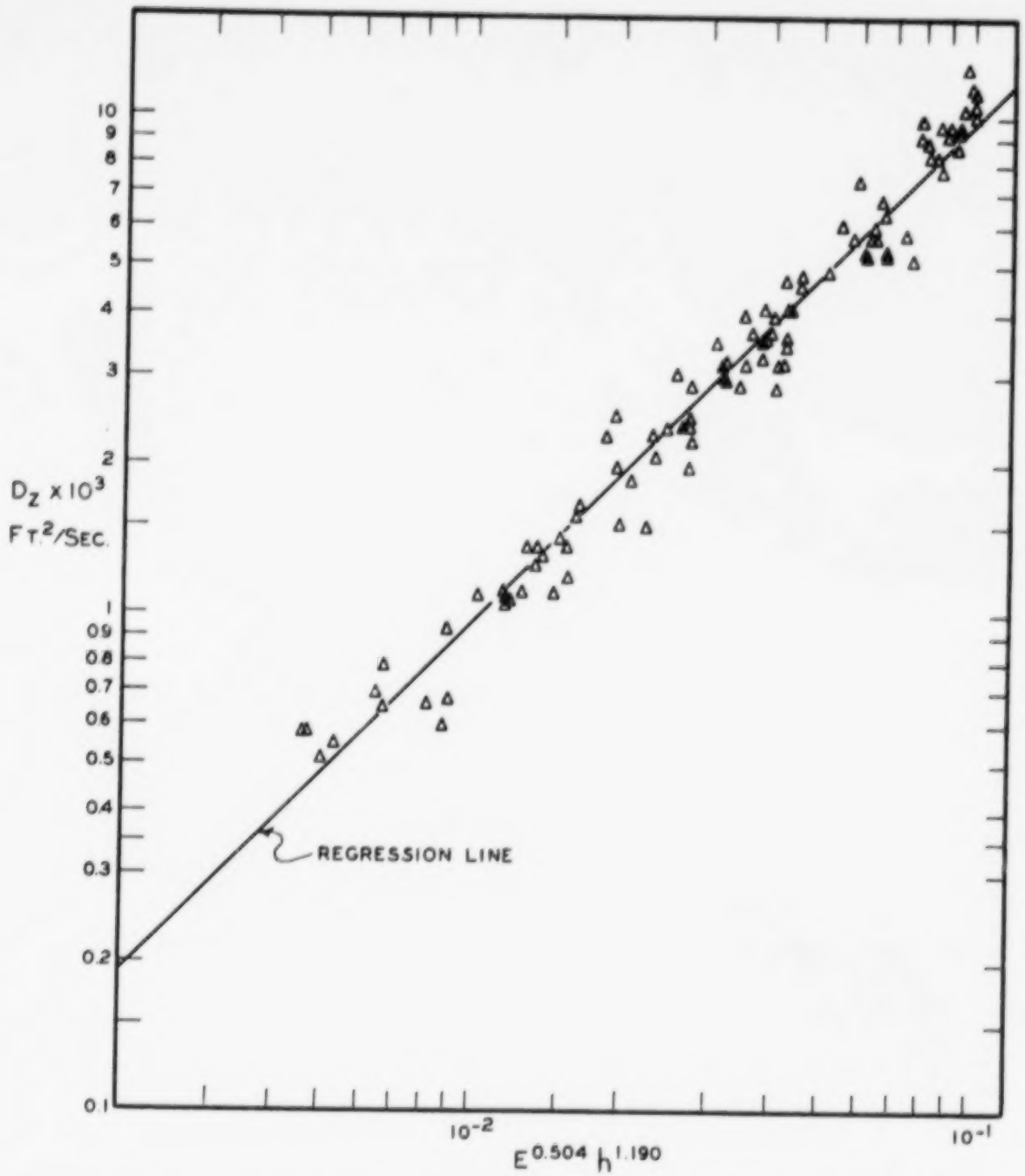

FIGURE 14: RELATION BETWEEN D_z AND THE ENERGY DISSIPATION

the water surface to the top of the expanded wire mesh rather than the measured depth for the scale factor. Upon reflection, this is indeed logical, because presumably, h represents the diameter of the largest eddy, and large eddies cannot extend into the area occupied by the mesh.

The remaining difference in the constants is presently believed to be due to the influence of bottom roughness. Manning's roughness coefficient was calculated for each run of both the California and Vanderbilt channels and the Vanderbilt channel has a greater roughness coefficient. The difference is most pronounced at shallower depths and is caused by a differential in thickness, or height, of the expanded wire mesh laid on the bottom to produce uniform turbulence, the Vanderbilt mesh being thicker.

The preliminary results of this phase of the study are presented on Figures 15 and 16 which indicate a most promising line of future endeavor.

It should be noted that all of the previously described measurements will be conducted such that the energy expenditure per unit mass of fluid can be computed, thus allowing further investigation of this phenomenon.

7. Mixing under Stratified Flow Conditions

An unusual opportunity to utilize the tracer techniques described herein resulted in a practical application of the mixing coefficient determination in a real water pollution investigation.

The problem presented was to demonstrate the existence of stratified flow conditions and the resulting inhibition of vertical mixing caused by the discharge of a heated effluent from a steam generating plant.

Figures 17 through 19 demonstrate centerline temperature profiles taken on a stretch of river which exists in the backwater of a manmade impoundment. It was required to demonstrate rather conclusively that the stratification caused by the heated condenser water was considerably reducing the waste assimilative

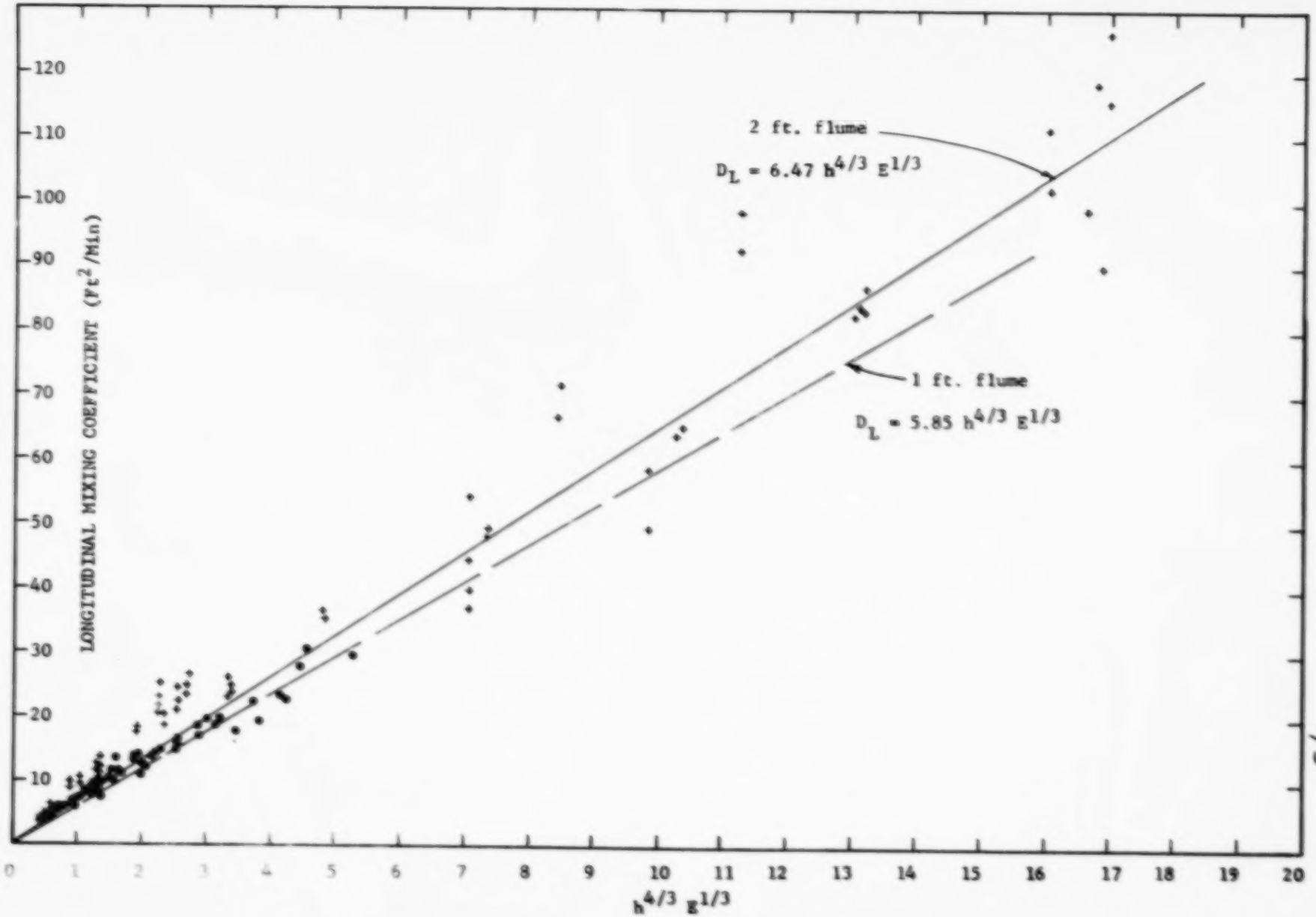

FIGURE 15: KOLMOGOROFF'S RELATIONSHIP FOR TWO FLUMES

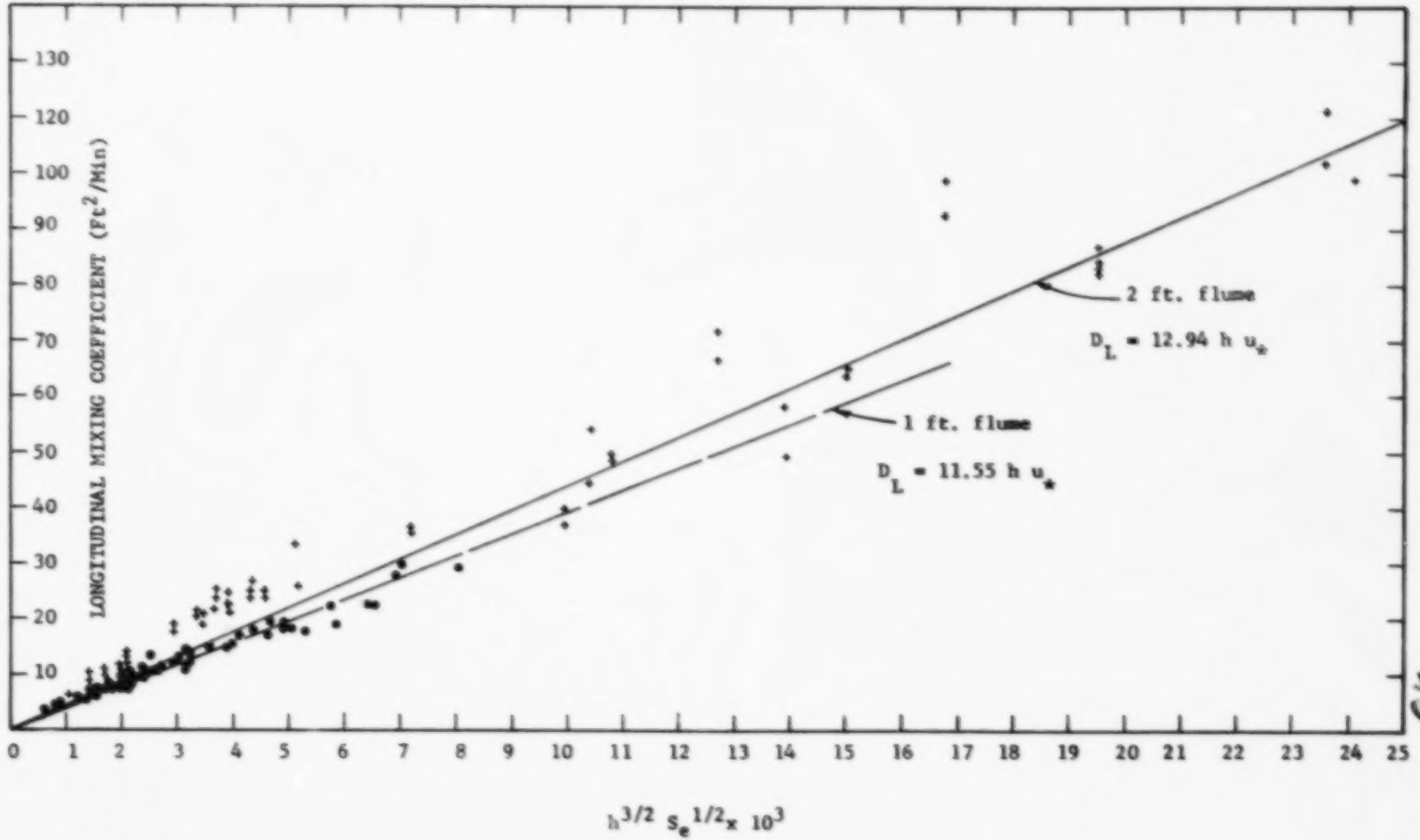

FIGURE 16: RELATIONSHIP BETWEEN SHEAR VELOCITY AND THE MIXING COEFFICIENT

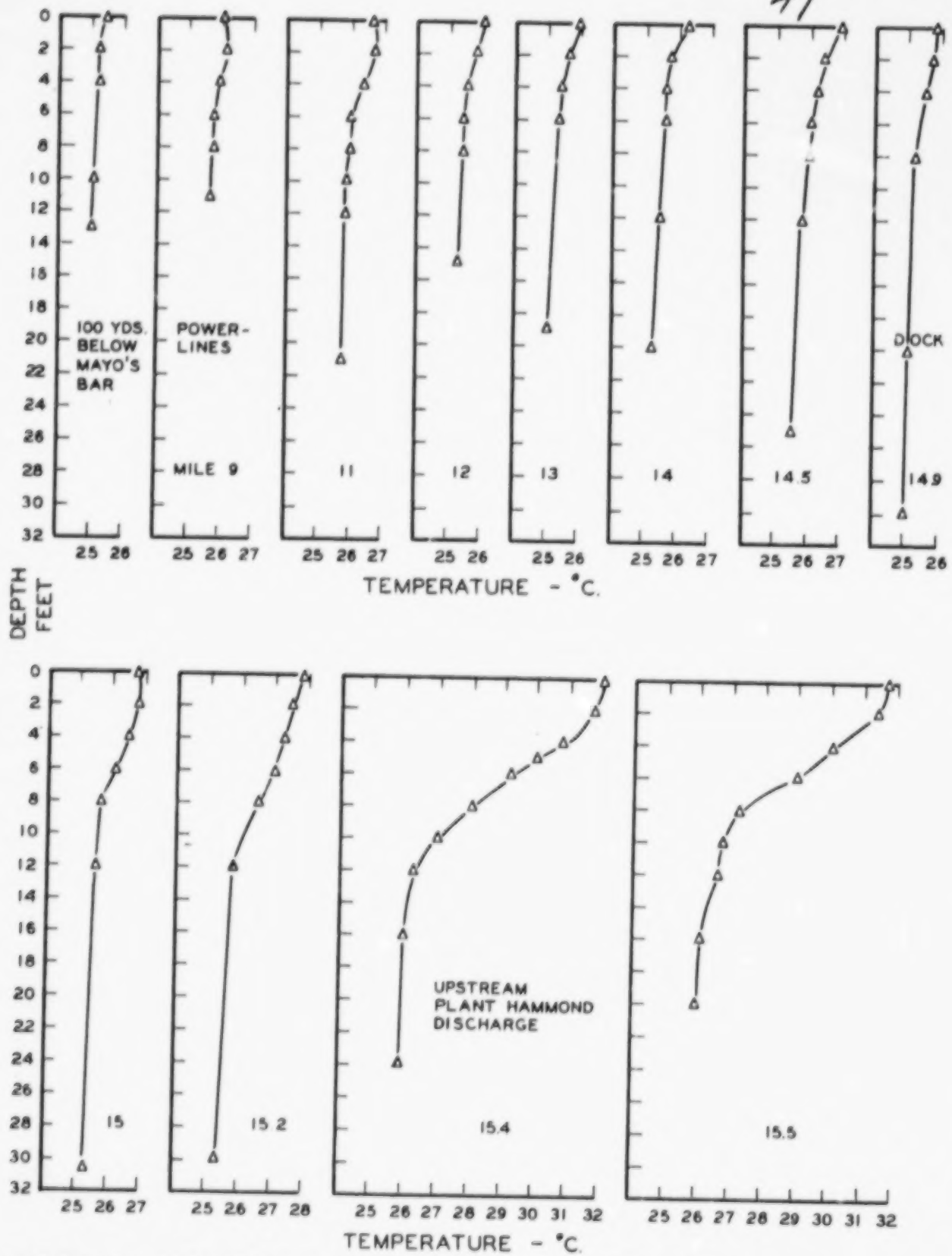

FIGURE 17: TEMPERATURE PROFILES - 4 SEPT. 1963

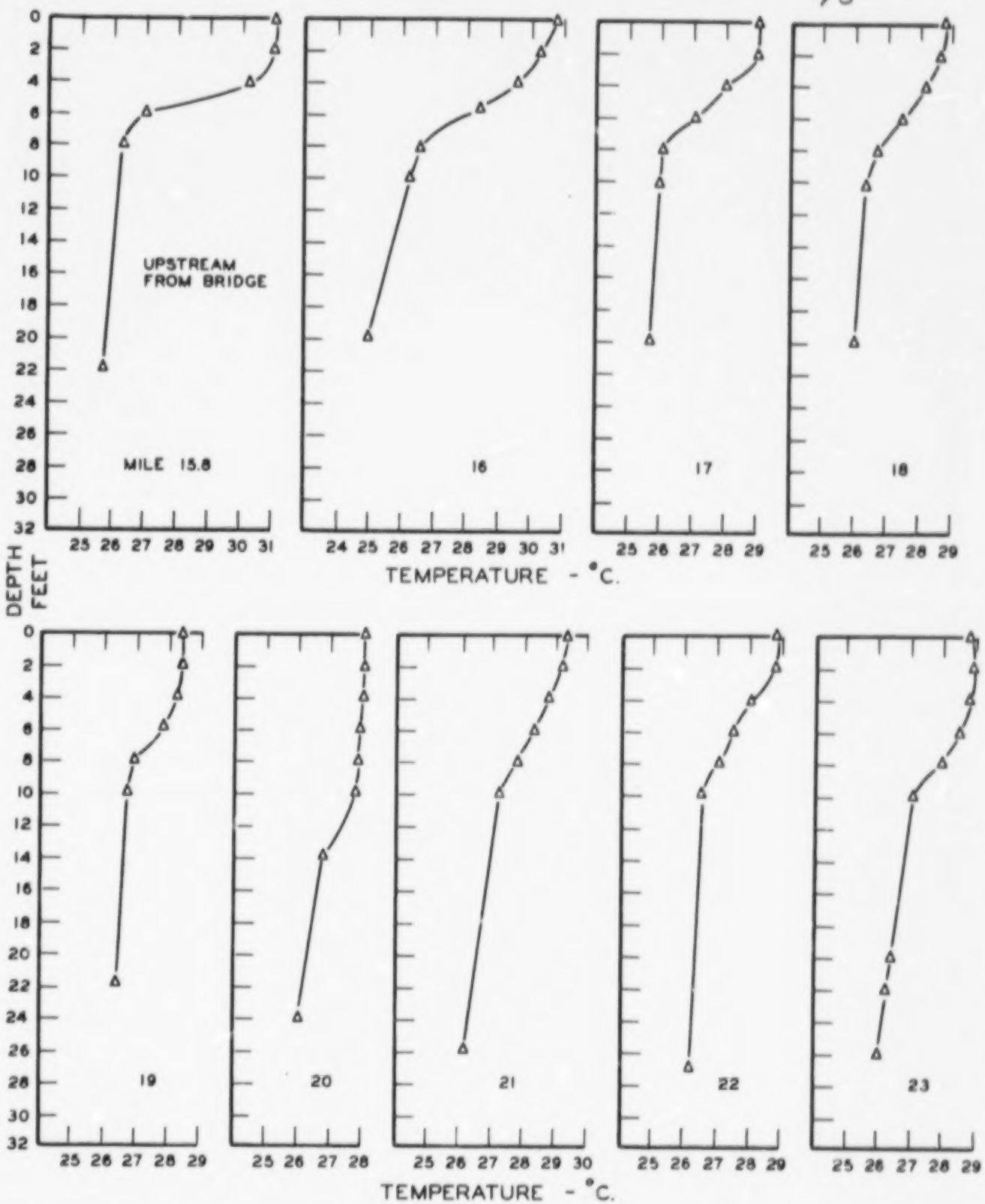

FIGURE 18: TEMPERATURE PROFILES - 4 SEPT. 1963

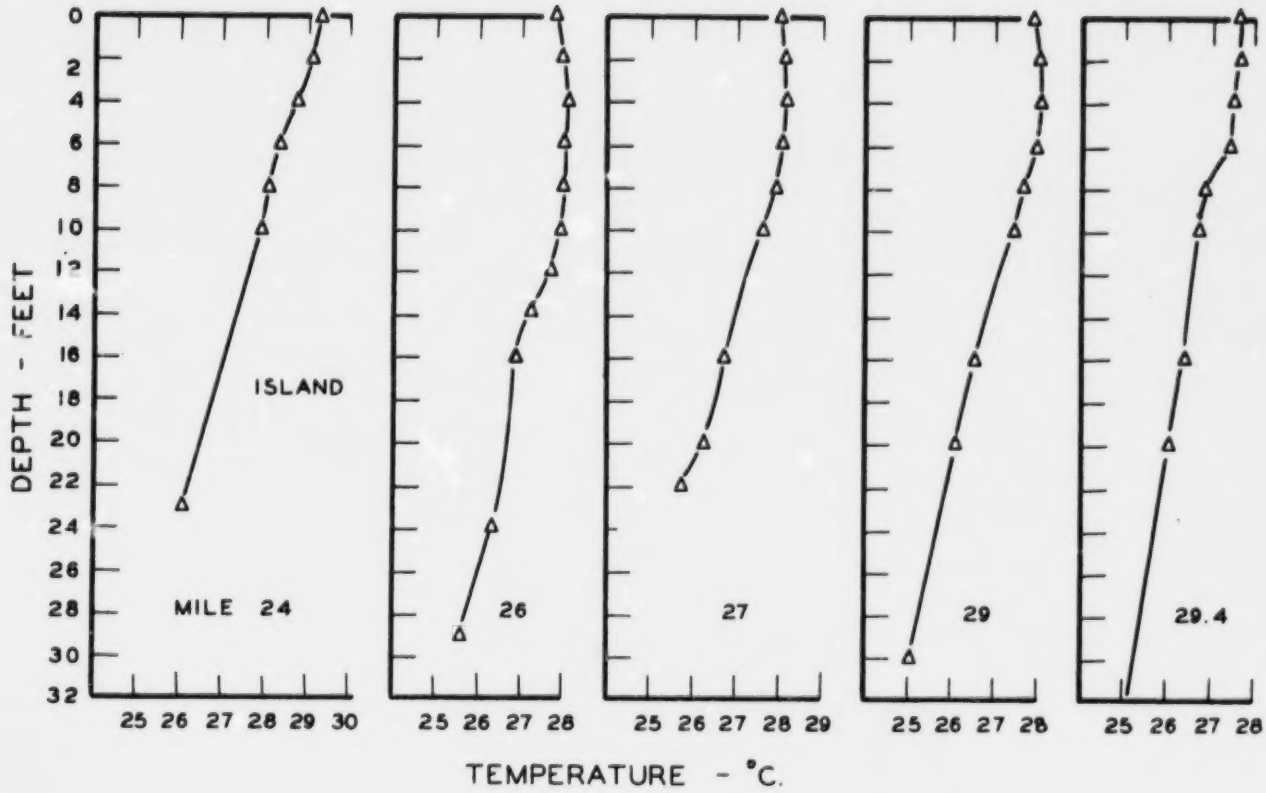

FIGURE 19: TEMPERATURE PROFILES - 4 SEPT. 1963

capacity of the stream by the resulting layer effect which prevents material contained in the lower layer from taking advantage of the dilution, dissolved oxygen and reaeration capacity in the upper layer.

A mass of Rhodamine "B" and a mass of gold 198 were injected essentially instantaneously into a diffuser pipe that extends across the river in question. The mass of tracer was then followed downstream utilizing a portable scintillation counger for the radioactive gold and a Fluorometer for the fluorescent Rhodamine B detection.

The time-concentration profile of the injected tracer material was followed for a considerable distance downstream, and while difficulties encountered during the survey yielded some scatter of the points, the resulting flow-through curves yielded important information concerning the lack of vertical mixing as well as the detention period for various reaches of the river.

Examination of Figure 20 demonstrates that the greater mass of tracer material did not mix with the upper stratified layer as far as three miles downstream from the point of injection. In order to determine relative orders of magnitude of the mixing taking place in these two layers, necessary assumptions were made such that a relative longitudinal mixing coefficient could be determined for both layers of the stratified flow.

The results of this analysis yielded a value of D_L = 30 ft^2/sec for the upper layer and 12 ft^2/sec for the lower layer. While the assumptions necessary for these calculations may be somewhat questionable, the difference in orders of magnitude of the mixing taking place in the two layers appears to be significant and certainly substantiates the existence of two different flow regimes.

It should be noted that this investigation was conducted during November, 1963 when the air temperature was colder, the water temperature was colder and

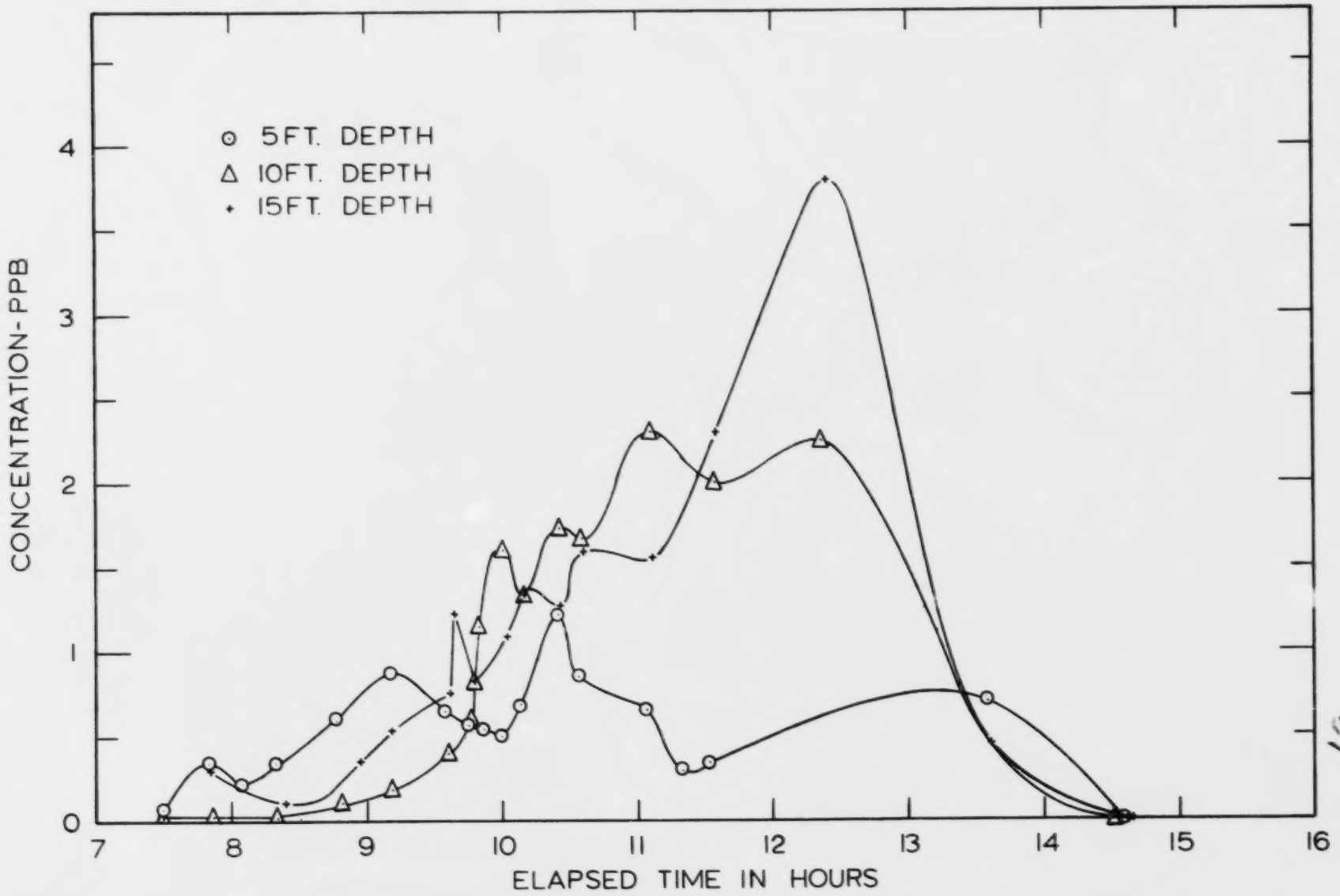

FIGURE 20: RHODAMINE "B" FLOW-THROUGH CURVE (MILE 18)

the stream flow was higher than that occurring during the critical time for waste assimilative capacity of the river. It should be obvious even to the casual observer, that critical summer conditions would yield a much more stable stratified flow condition and for an even greater distance, thus compounding the problem.

The usefulness of these techniques and the ever-increasing problems being created by the progressive development of our water resources demonstrates the need for refinement of tracer methodology. Future plans for these studies include the analysis and field scale investigations of stratified flow phenomenon as related to waste assimilative capacity.

8. Present Work and Potential of Project

Because the initial phases of these investigations were largely involved with equipment design and refinement of methodology, the major portion of the experimental data will be obtained in the ensuing months. It is expected that sufficient data will be produced by October of 1964 such that the desired analyses can be performed, both in the laboratory flume and in the selected TVA rivers.

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APPENDIX A

APPLICATION OF FREQUENCY RESPONSE TECHNIQUES TO THE ANALYSIS OF TURBULENT DIFFUSION PHENOMENA

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Paper Presented

To

19th Annual

Industrial Waste Conference

May 7, 1964

Purdue University
Lafayette, Indiana

SUMMARY

This paper presents a review of the pulse testing method for dynamic analysis of systems. Experimental pulse data is reduced to frequency domain information by numerically computing the Fourier transform. A digital computer is necessary for the data reduction. The procedure by which the frequency domain information is found is presented in the paper, and a brief description of the FORTRAN data reduction program for the I.B.M. 7072 computer is given.

Simultaneous mass transport of dissolved or suspended material can be described by the following equation:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x}$$

Two solutions of this equation are presented in this paper. One solution, due to Levenspiel (14), is given for a mass of material rapidly injected at the origin of the test system boundary. The second solution, by Clements (4), is applicable when both the input and output concentrations are measured in the pipe. Under such conditions the pulse testing method may be used for data reduction. Levenspiels' solution is in the time domain while Clements' of necessity presents a frequency domain equation.

A mathematical modeling procedure is described which uses the integral of the squared error as a measure of deviation. This parameter is minimized by a non-linear least squares procedure due to Marquardt (18). This technique simultaneously presents the statistical best values of the model parameters and the standard error of estimate, a measure of how well the model describes the system.

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Application of both the pulse testing techniques and the modeling procedure was made to the problem of axial mixing in a 35 foot long, one inch diameter, Pyrex glass pipe. Sodium chloride pulses were injected and the input and output recorded through electrical conductivity bridges. The results of the investigation are presented in this paper. The study showed that at higher Reynolds Number the standard error of estimate is of the same order of magnitude as the experimental error. Thus, the model is a near perfect fit in the higher Reynolds Number region. It was found that over the range of Reynolds Number of 3×10^3 through 3×10^5 the data could be correlated by the following expression:

$$Pe = -1958 + 694 \log Re$$

This relationship is somewhat in disagreement with Taylor (9) whose study was conducted in a smaller range of Reynolds Number. Further study is required to confirm the relationship presented in this paper.

APPENDIX B

1. List of publications supported in whole or in part by this grant.

   a. Hays, J.R., Schnelle, K.B., and Krenkel, P.A., "Application of Frequency Response Techniques to the Analysis of Turbulent Diffusion Phenomena," 19th Annual Industrial Waste Conference, Purdue Univ., 1964.

   b. Hays, J.R., "One-Dimensional Diffusion Model Studies in a Long Pipe," M.S. Thesis, Vanderbilt University, 1964.

   c. Driver, E.E., "The Effect of Impoundments on Waste Assimilative Capacity," M.S. Thesis, Vanderbilt University, 1964.

   d. Krenkel, P.A., discussion to paper by D.R.F. Harleman entitled "Significance of Longitudinal Mixing in Pollutional Analysis of Estuaries" presented at 2nd Intl. Conf. on Water Pollution, Tokyo, Japan, 1964.

   e. Krenkel, P.A., "Effects of Stratified Flow on Water Quality," to be presented at ASCE Water Resources Conf. in Mobile, Alabama, 1965.

   f. Krenkel, P.A., "Effects of Impoundments on Waste Assimilative Capacity" to be presented at Water Poll. Control Fed. Meeting Bal Harbour, Florida, 1964.

   g. Schnelle, K.B., Hays, J.R., Krenkel, P.A., "Experimental Results of Frequency Response Techniques in Water Pollution Studies," to be presented at AIChE Meeting, Houston, Texas, 1965.

2. Participating Professional Personnel and time expended on this research.

   The following professional personnel have contributed to the research effort during the report period.

   Krenkel, Peter A., Associate Professor and Director, Sanitary and Water Resources Engineering; 70% time summers; 10% time academic year.

   Schnelle, Karl B., Associate Professor of Chemical Engineering; 70% time summers; 10% time academic year.

   Hays, James R., Graduate Student, Chemical Engineering; full time summer; 50% time academic year.

   Driver, Edward E., Graduate Student, Civil Engineering; full time summer; 50% time academic year.

   Morris, James C., Graduate Student, Civil Engineering; full time summer; 50% time academic year.

Thackston, Edward L., Graduate Student, Civil Engineering; 10% time during past year at no cost to the grant.

Tidwell, Greer C., Graduate Student, Civil Engineering; full time summer 1962 and summer 1963.

INTRODUCTION

Turbulent mass transport of dissolved or suspended material in a carrier fluid occurs in a great many problems of engineering interest. In more idealized situations, such as natural gas and gasoline transport by pipelines, adequately descriptive solutions can be found. However, for complex systems, such as open channel flow or natural streams and rivers, solution of the describing equations becomes difficult and impractical. The satisfactory formulation of approximate phenomenological models for these more complicated cases involves a step by step procedure beginning with an experimental study of the limits of application of a one dimensional transport model to simple pipe flow. On the basis of these results the study should be expanded to include an open channel flow laboratory model and, finally, natural streams. This paper will be concerned primarily with the development of a dynamic testing technique and mathematical modeling procedure to compare proposed models to a physical system. Application of these techniques to the problem of axial mixing in a one inch diameter, 35 foot long glass pipe, will be discussed briefly.

HISTORICAL BACKGROUND

Simultaneous mass transport by bulk flow and turbulent mixing can be described in the one dimensional case by the partial differential equation

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} \qquad (1)$$

where x is the space coordinate, t is time, C is the concentration, D_L is the longitudinal mixing coefficient, and u is the velocity. The term $D_L \frac{\partial^2 c}{\partial x^2}$ accounts

for the turbulent mixing transport and $u \frac{\partial C}{\partial x}$ is the bulk transport term. Solutions to this equation for a number of boundary conditions have been given in the literature (1,2,3,4,6,14,20). Solutions for equation 1 extended to two dimensions to account for turbulent transport in the radial direction have been given by Bischoff and Levenspiel (2). A constant radial mixing coefficient was assumed by Bischoff. No solutions are known that take into account the variation in the radial mixing coefficient with radius. It is doubtful that a rigorous solution can be found for stream flow where both mixing and bulk transport mechanisms are evident in three dimensions and where other complicating phenomena are present.

In a series of articles, Taylor reported the results of an investigation of the application of equation 1 as a longitudinal mixing model. The first paper (15) was a theoretical development showing that this relatively simple model gives valid results at very low Reynolds numbers where other phenomena not considered by the model, such as velocity profile distortion and molecular diffusion, are important. This theoretical conclusion was experimentally verified.

The second article (16) was concerned with the derivation of a relationship between the axial mixing coefficient in turbulent flow and the Reynolds number. The development was based upon theoretical turbulent velocity profiles. A few experiments were carried out in a limited range of Reynolds numbers.

The third article (17) demonstrated a method of measuring molecular diffusion occuring simultaneously with laminar flow.

Most experimental measurements of longitudinal dispersion have been carried out for special purposes under less than ideal circumstances. Hull and Kent (12) used a radioactive tracer to measure dispersion in a pipeline through which crude oil was flowing. Davidson et. al. (7) performed essentially the same experiment

using hydrogen as a tracer in a refinery gas pipeline. Taylor (16) points out that fittings, valves, bends in the pipes, etc., make it difficult to compare such data to results predicted by theory.

It is common practice to determine the axial mixing coefficient by measuring the time during which the tracer pulse is greater than one half its maximum value, or by measuring the maximum value of the tracer pulses at two downstream stations, or by calculating the second moment of the tracer pulse. The axial mixing coefficient is directly related to all of these quantities (14,16). In each method the input must be an instantaneous injection. It is a severe disadvantage that none of these methods give any information about the limits to which the assumed model describes the real situation. If the model does not "fit", the mixing coefficient is not meaningful.

PULSE TESTING METHOD

Most solutions of the differential equations describing mixing phenomenon are more easily obtained in the frequency domain. Time domain solutions can usually be found for only idealized boundary conditions such as an instantaneous injection. For arbitrary boundary conditions it may be impossible to obtain time domain solutions to these differential equations, whereas the frequency domain solutions for these equations are relatively easily found. Thus an efficient procedure that would lead to frequency domain information is a highly desirable tool. Moreover, if such a test could accept an arbitrary input, it would remove the instantaneous injection restriction required by the test procedures discussed in the last section.

Pulse testing is a procedure that satisfies these requirements in that any arbitrary input pulse may be used. The method requires the recording of both

the input and output pulse which can be reduced, through Fourier analysis, to frequency domain information. Several articles of a review nature have appeared in the literature recently. These articles will be of interest to the reader considering the use of the pulse method. Particular reference is made to Clements and Schnelle (5) who presented details of certain theoretical and practical aspects of pulse testing, and to Hougen and Walsh (11) and Dreifke, Hougen, and Mesmer (8) who presented Bode plots of the results of numerous pulse tests on various chemical process type systems in addition to contributing theoretical information.

This paper will discuss the pulse testing method and its application to frequency domain modeling of the axial mixing problem.

Transfer Function

The transfer function will be defined for the purpose of this paper in reference to a system that can be described by a linear differential equation. A simple mixing tank satisfies the above linearity requirement. For such a tank the following differential equation can be written

$$V \frac{dC_o}{dt} = QC_i - QC_o \qquad (2)$$

where Q is the flow through the tank, V is the volume of the tank, C_i is the inlet concentration, and C_o is the outlet concentration. Laplace transforming this equation assuming C_o is zero at time zero results in the following equation

$$(T s + 1)\, C_o(s) = C_i(s) \qquad (3)$$

where $T = V/Q$. The ratio of the transformed output concentration to the transformed input concentration is the transfer function and is given by

$$G(s) = \frac{C_o(s)}{C_i(s)} = \frac{1}{Ts + 1} \qquad (4)$$

Note that the only parameters in the right hand side of equation 4 are Q and V which are system characteristics and not functions of the input. Thus, by taking the ratio of the transformed output to the transformed input, a function is produced which depends only on the system in question and is independent of the form of the input. Knowledge of the transfer function implies that the system response can be computed for any given input. Moreover, only the system parameters and a mathematical model must be known to be able to derive the transfer function.

Frequency Response by Sinusoidal Methods

Frequency response of a system can be determined experimentally by imposing a constant frequency, sinusoidally varying input on the system. When the system reaches steady state the input and output variables are recorded as two sinusoidal traces. The magnitude ratio and phase angle at the given frequency are determined from the recordings with a pair of dividers and other suitable measuring instruments. A whole range of frequencies is then investigated and plots of frequency versus magnitude ratio and phase angle are constructed. These plots are called Bode plots. The same analysis could have been made analytically by solving equation 2 for a sinusoidal input. However, a mathematical shortcut exists. Replacing s by $j\omega$ gives the same information as if the original differential equation had been solved for a sinusoidal input. The magnitude ratio and phase angle may be computed from the resultant complex number. The mixing tank equation can be used to illustrate the point as follows. Replace s by $j\omega$ in equation 4

$$G(j\omega) = \frac{C_o(j\omega)}{C_i(j\omega)} = \frac{1}{j\omega T + 1} \qquad (5)$$

This complex number can then be resolved into a magnitude ratio (M.R.) and phase

angle (P.A.) given by

$$M.R. = \frac{1}{1 + (\omega t)^2} \tag{6}$$

$$P.A. = \arctan(-\omega t) \tag{7}$$

The Bode plot could now be constructed analytically from equations 6 and 7. Note also that equation 5 is the frequency domain solution of the mixing tank differential equation for any arbitrary input.

Frequency Response by Pulse Methods

Returning to the definition of the transfer function given by equation 4, the output-input ratio can be rewritten in terms of the definition of the Laplace transform

$$G(s) = \frac{C_o(s)}{C_i(s)} = \frac{\mathcal{L}[C_o(t)]}{\mathcal{L}[C_i(t)]} \tag{8}$$

or more generally for any input-output functions

$$G(s) = \frac{Y(s)}{X(s)} = \frac{\int_0^\infty y(t)e^{-st}dt}{\int_0^\infty x(t)e^{-st}dt} \tag{9}$$

where x (t) is the input and y(t) is the output function.

Now, as before replace s by $j\omega$ and note that in this form the transfer function

$$G(j\omega) = \frac{Y(j\omega)}{X(j\omega)} = \frac{\int_0^\infty y(t)e^{-j\omega t}dt}{\int_0^\infty x(t)e^{-j\omega t}dt} \tag{10}$$

is a Fourier transform. This form of the transfer function requires only that the input and output trace be closed curves. Therefore, the input and output

are not restricted to sinusoidal forms and may be arbitrary time functions such as closed pulses.

Suppose that the input and output are not given by analytical functions but are recordings resulting from a physical test. If the recordings are closed pulses as shown in Figure 1, the Fourier transforms cannot be found by analytical integration and a method must be developed to numerically evaluate the integrals

$$\int_0^\infty y(t)e^{-j\omega t}dt \qquad \text{and} \qquad \int_0^\infty x(t)e^{-j\omega t}dt$$

It is convenient to rewrite the term $e^{-j\omega t}$ according to Eulers relation $e^{-j\omega t} = \cos(\omega t) - j\sin(\omega t)$ and the Fourier transforms can be rewritten as

$$G(j\omega) = \frac{\int_0^{Ty} y(t)\cos(\omega t)dt - j\int_0^{Ty} y(t)\sin(\omega t)dt}{\int_0^{Tx} x(t)\cos(\omega t)dt - j\int_0^{Tx} x(t)\sin(\omega t)dt} \tag{11}$$

The infinite limits on equation 10 have been replaced by Tx and Ty, the end of the closed pulses.

If

$$A = \int_0^{Ty} y(t)\cos(\omega t)dt \tag{12}$$

$$B = \int_0^{Ty} y(t)\sin(\omega t)dt \tag{13}$$

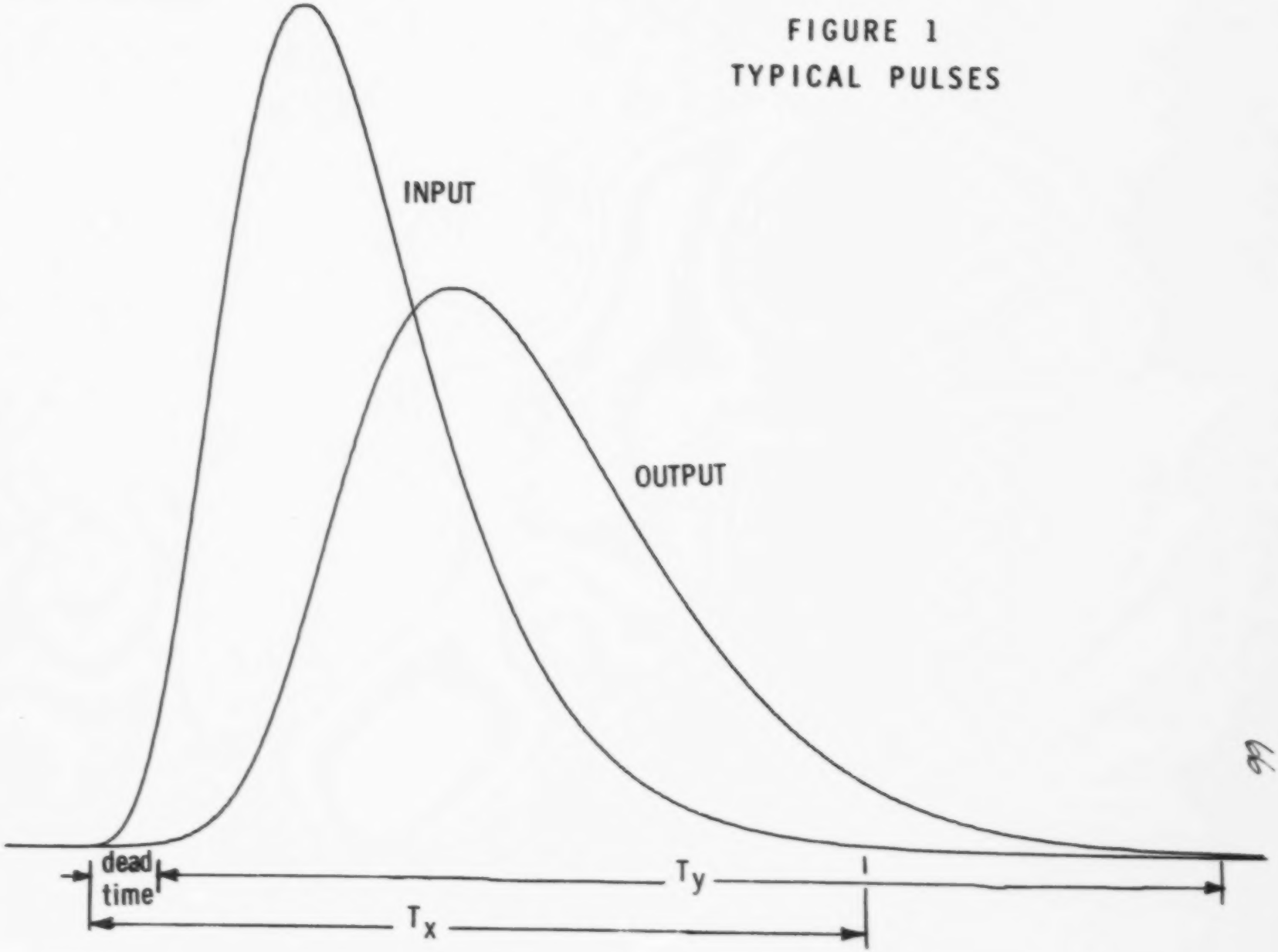
$$C = \int_0^{Tx} x(t)\cos(\omega t)dt \tag{14}$$

$$D = \int_0^{Tx} x(t)\sin(\omega t)dt \tag{15}$$

Equation 11 can be rewritten as

$$G(j\omega) = \frac{A - jB}{C - jD} \tag{16}$$

FIGURE 1
TYPICAL PULSES



If $G(j\omega)$ is written in terms of a magnitude ratio and phase angle

$$G(j\omega) = \text{M.R.} \quad e^{-j\left[\text{P.A.}(\omega)\right]} \tag{17}$$

Then comparing equations 11 and 17 it can be shown that

$$\text{M.R.} = \sqrt{\frac{A^2 + B^2}{C^2 + D^2}} \tag{18}$$

$$\text{P.A.} = \arctan \left[\frac{AD - BC}{AC + BD}\right] \tag{19}$$

Numerical Procedure.

In the usual case, common numerical techniques could be directly applied to the integrands such as $y(t) \cos(\omega t)$ appearing in the equations 12,13,14 and 15. Thus, the integrals could be evaluated by a quadrature formula such as the trapezoidal rule or Simpson's Rule. These formulas are not adequate, however, for the evaluation at higher frequencies of integrals of the type in equations 12 through 15. The difficulty lies in not being able to numerically describe the high frequency oscillations of the sinusoidal function using a reasonable number of panels. However, the pulse functions, $x(t)$ and $y(t)$, can be satisfactorily approximated by a polynomial over a small panel. Then the approximation curve can be multiplied by the sinusoidal function and analytically integrated over each panel. The value of the integral is obtained by summing the value of the integrals from the individual panels. Such a technique was used by L. N. G. Filon (9).

Estimate of Reliability of the Computation

The normalized frequency content, $S_n(\omega)$, is a measure of harmonic content of each pulse. For the input pulse, it is an indication of the degree to which the system is excited. For the output pulse, it indicates the degree to which the

system responded to the input. When either the output or the input normalized frequency content approaches the order of magnitude of the experimental error, the reliability of the calculated values of magnitude ratio and phase angle degenerates. The input or output normalized frequency content can be calculated as follows from the quantities A, B, C, and D defined above:

$$S_{xn}(\omega) = \frac{\left| \int_0^{Tx} x(t) e^{-j\omega t} dt \right|}{\left| \int_0^{Tx} x(t) e^{j(o)} dt \right|} \tag{20}$$

$$S_{xn}(\omega) = \frac{\left(\sqrt{C^2 + D^2}\right)_\omega}{\left(\sqrt{C^2 + D^2}\right)_{\omega=o}} = \frac{\left(\sqrt{C^2 + D^2}\right)_\omega}{(C)_{\omega=o}} \tag{21}$$

Similarly for the output pulse y(t):

$$S_{yn}(\omega) = \frac{\left(\sqrt{A^2 + B^2}\right)_\omega}{\left(\sqrt{A^2 + B^2}\right)_{\omega=o}} = \frac{\left(\sqrt{A^2 + B^2}\right)_\omega}{(A)_{\omega=o}} \tag{22}$$

Figure 2 further illustrates the concept of frequency content by comparing ten pulses that can be expressed analytically on a plot of normalized frequency content versus frequency.

Digital Computer Program.

While it is possible to hand calculate or graphically process pulse data to magnitude ratio, phase angle, and frequency content, it is obviously not technically feasible. Thus it is necessary to make use of a digital computer for the data reduction.

A pulse to frequency response program has been written in Basic FORTRAN language for the I.B.M. 7072 computer. The program allows a wide latitude in the

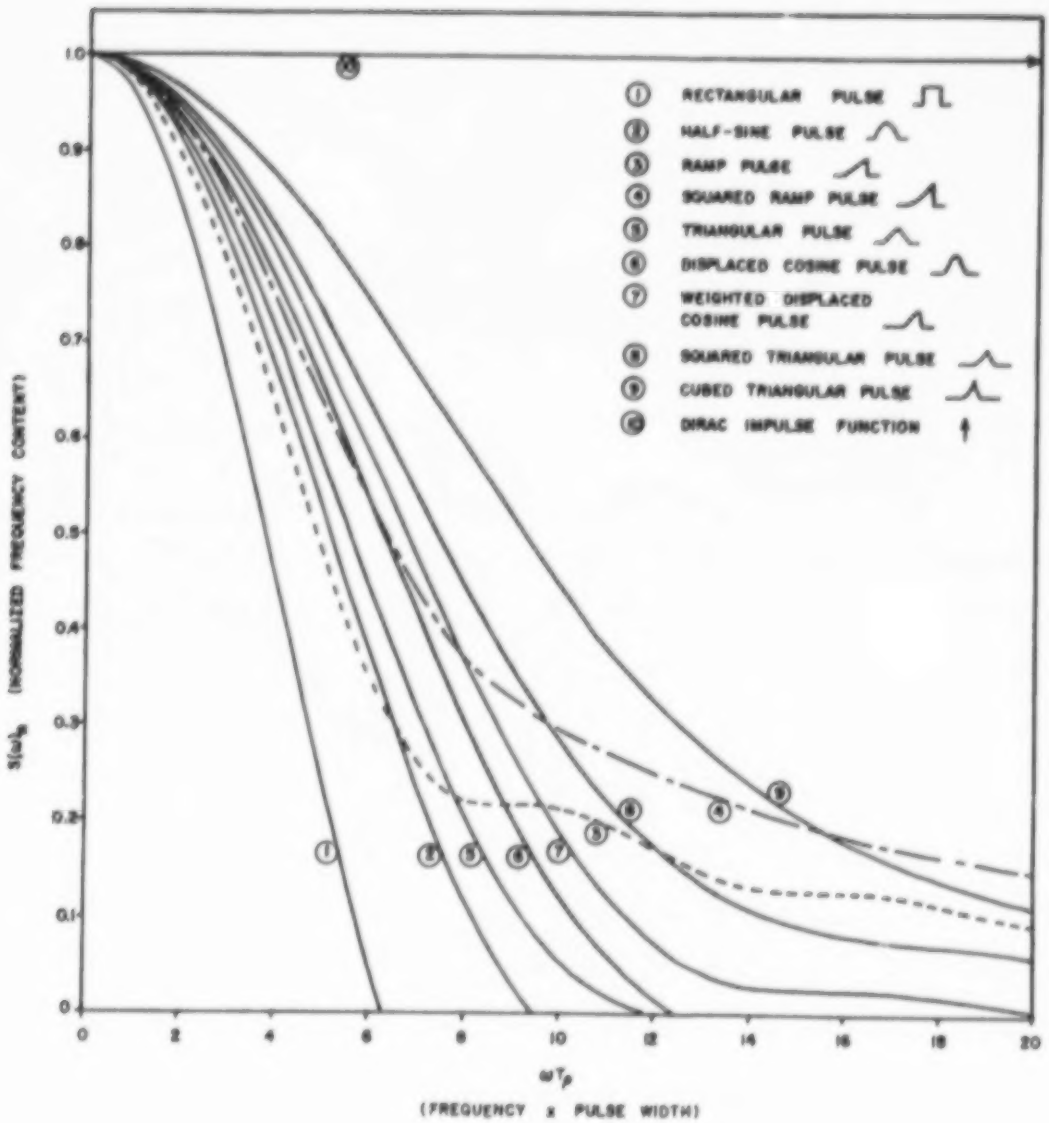


FIGURE 2

NORMALIZED FREQUENCY CONTENT OF TEN ANALYTICAL PULSES

form of the input information. For example, closely spaced points may be read from pulses over regions of rapid change and more widely spaced points over regions of gentle change. Provision is made for the addition of a raw data processor if desired. The basic output of the program is a list of frequency domain quantities such as magnitude ratio, phase angle, etc., tabulated at desired frequencies. A plotting option has been provided that plots both the input and output pulses on the same coordinates. An option for plotting magnitude ratio versus frequency is also provided. The program can be used on any computer with a basic FORTRAN compiler and about a 5000 word memory. A program description is available from the authors upon request.

TWO SOLUTIONS OF THE DIFFUSION EQUATION

The distribution in time and space of a soluble tracer in a stationary, homogeneous solvent depends solely upon molecular transport. If this molecular transport is described by Fick's Law of diffusion there results the partial differential equation

$$\frac{\partial C}{\partial t} = \nabla^2 DC = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \qquad (23)$$

where C is concentration, t is time, x,y,z, are the space coordinates, D is diffusivity, and ∇ is the Laplacian operator.

If space is restricted to one coordinate, equation 23 can be rewritten as

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} \qquad (24)$$

The analogy between longitudinal mixing on the macroscopic scale in pipe flow and molecular diffusion has been pointed out by a number of authors. Levenspiel

(2) discusses the literature pertinent to this analogy. To implement this idea, D_x is replaced by D_L, the longitudinal mixing coefficient, and equation 24 is modified to include bulk flow. This gives

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} \tag{25}$$

where u is the longitudinal velocity. An attempt to apply this equation to pipe flow involves the extension to two more dimensions and implies complete homogeneity in these dimensions at all time. In terms of cylindrical coordinates, this restriction in the angular direction is easily met for most situations. However, concentration gradients may occur in the radial direction according to the type of flow.

Equation 25 may be written in dimensionless form as

$$\frac{\partial C}{\partial \theta} = \frac{1}{Pe} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} \tag{26}$$

where

$$\theta = \frac{u}{L} t \qquad Z = \frac{x}{L} \qquad Pe = \frac{uL}{D_L}$$

L = characteristic length

D_L = longitudinal mixing coefficient

Pe = Peclet number

Two solutions of equation 26 are of particular importance. One has been developed by Clements (4), and the other is suggested by Levenspiel (2,14). Clements developed a Laplace domain transfer function between an arbitrary input concentration measured as a function of time a z = 0, and the resulting output concentration as a function of time at a given z. The boundary conditions were

$$C(z,o) = 0 \tag{27}$$

$$\lim_{Z \to \infty} \quad C(Z,\theta) = 0 \tag{28}$$

$$C(o,\ \theta) = C_{1\ in}(\theta) \quad \theta > 0 \tag{29}$$

The transform solution is

$$\tilde{C}\ (Z,S) = \left[\tilde{C}_{1\ in}\ (S_n)\right] \exp\left[\left(\frac{1 - \sqrt{1 + 4\ S_n/Pe}}{2/Pe}\right) Z\right] \tag{30}$$

where S_n is a dimensionless Laplace transform variable and $\tilde{C}$ refers to transformed variables. This equation may be written

$$\tilde{C}(Z,\ S_n) = \left[\tilde{C}_{1\ in}(S_n)\right]\ \left[G_1(Z,S_n)\right] \tag{31}$$

where $G(Z,S_n)$ is the Laplace transfer function. Inversion to the time domain gives

$$C(Z,\theta) = \left[C_{1\ in}(\theta)\right] * \left[g_1(Z,\theta)\right] \tag{32}$$

where * indicates convolution and $g_1(Z,\theta)$ is the inverse transform of $G_1(Z,S_n)$. Inversion of $G_1(Z,S_n)$ gives

$$g_1(Z,\theta) = \frac{Z}{\theta}\sqrt{\frac{Pe}{4\pi\theta}}\ \exp\left[-\frac{Pe(Z-\theta)^2}{4\theta}\right] \tag{33}$$

This equation can be converted to dimensional coordinates by use of the following transform relation

$$\left(\frac{u}{L}\right)\ g_1\left(Z,\ \frac{ut}{L}\right) \quad \text{transforms to} \quad G\left(Z,\ \frac{L}{u}\ S\right) \tag{34}$$

application of this relation gives

$$g_1(x,t) = \frac{x}{t}\sqrt{\frac{1}{4\pi D_L t}}\quad \exp\left[-\frac{(x-ut)^2}{4D_L t}\right] \tag{35}$$

To obtain the frequency domain solution substitute $j\omega_n$ for S_n in equation 30. The quantity ω_n is a normalized frequency given by

$$\omega_n = \left(\frac{L}{u}\right)\omega \tag{36}$$

Making this substitution gives

$$C(Z,\omega_n) = \left[C_1\ in(\omega_n)\right]\quad \exp\left[\left(\frac{1-\sqrt{1+\frac{4\,(j\omega_n)}{Pe}}}{2/Pe}\right)Z\right] \tag{37}$$

Defining

$$a = \frac{4\omega_n}{Pe} \qquad b = 1/2 \text{ arc tan } a \tag{38}$$

The magnitude ratio and phase angle can be found for the Clements' solution

$$M.R. = \exp\left\{\frac{Pe}{2}\left[1-(1+a^2)^{1/4}\cos(b)\right]\right\} \tag{39}$$

$$P.A. = -\frac{Pe}{2}\left[(1+a^2)^{1/4}\sin(b)\right] \tag{40}$$

A second solution is given by Levenspiel (14) for a mass of tracer M rapidly injected at x = 0. The boundary conditions are

$$C(x,o) = 0 \qquad \lim_{x\to\infty} C(x,t) = 0 \tag{41}$$

$$\lim_{\to 0}\left[\int_{-\infty}^{\infty} C(x,t)\,A\,dx\right] = M \tag{42}$$

The last condition is true for all time, but in particular it defines the boundary conditions at t = 0. Here A is the cross sectional area of the pipe. The

solution can be written

$$C(x,t) = \frac{M}{A\sqrt{4\pi D_L t}} \exp\left[-\frac{(x-ut)^2}{4D_L t}\right] \tag{43}$$

The cross sectional area may be expressed as

$$A = V/L$$

where L and V are respectively the length and volume of the test section. Thus, at $x = L$, equation (43) can be written

$$\frac{C(L,t)}{Cavg} = \sqrt{\frac{Pe}{4\pi \frac{t}{(L/u)}}} \exp\left[-\frac{Pe\left(1-\frac{t}{(L/u)}\right)^2}{\frac{4t}{(L/u)}}\right] \tag{44}$$

where Cavg = M/V. It is the concentration that would be measured if the entire mass of the tracer were uniformly distributed in the test section volume, V. This is the form of Levenspiels solution most suitable for comparison of experimental response of a system to rapidly injected tracer. Note that the normalized concentration C(L,t)/Cavg is a function of only two parameters, Pe and L/u.

It should be well understood when each of the above solutions is applicable. Clements' solution should only be used when both input and output concentrations are measured inside the pipe. It should not be used for assumed inputs, such as a step or an inpulse input. In reality such drastic input concentration profiles can never be physically achieved. Usually an impulse or a step change in injection input is achieved and Levenspiel's solution is applicable.

Figure 3 shows how a typical injection impulse would look if concentration were measured both in the injection stream and in the pipe itself. Notice the relaxation tail that occurs in the concentration measured in the pipe. This is due solely to axial mixing. A similar effect is evident if a step change in injection input is used. Figure 4 shows this effect.

MATHEMATICAL MODELING

In mathematical modeling a set of equations is proposed to describe the system. The system and the model are excited under the conditions of interest and a comparison of the responses is made. It is difficult to generalize the preliminary steps in modeling as the considerations upon which the proposed models are based are usually unique to the particular problem. The reasons for considering a model may range all the way from an attempt to justify theoretical assumptions about a system to the desire for a predictive model that may be only empirical.

"Testing" the model includes both the design of the experiments to excite the system and gathering information about its response and the comparison of this response to that predicted by the model. Of course, in some cases it may not be feasible to perform experiments at will, and available information about the system must be accepted.

Any procedure concerned with the comparison of the system response to that described by the model should answer two questions quantitatively:

1. How well does the model describe the system?
2. What are the statistically best values of the model parameters?

To answer these questions a criterion of deviation must be established between

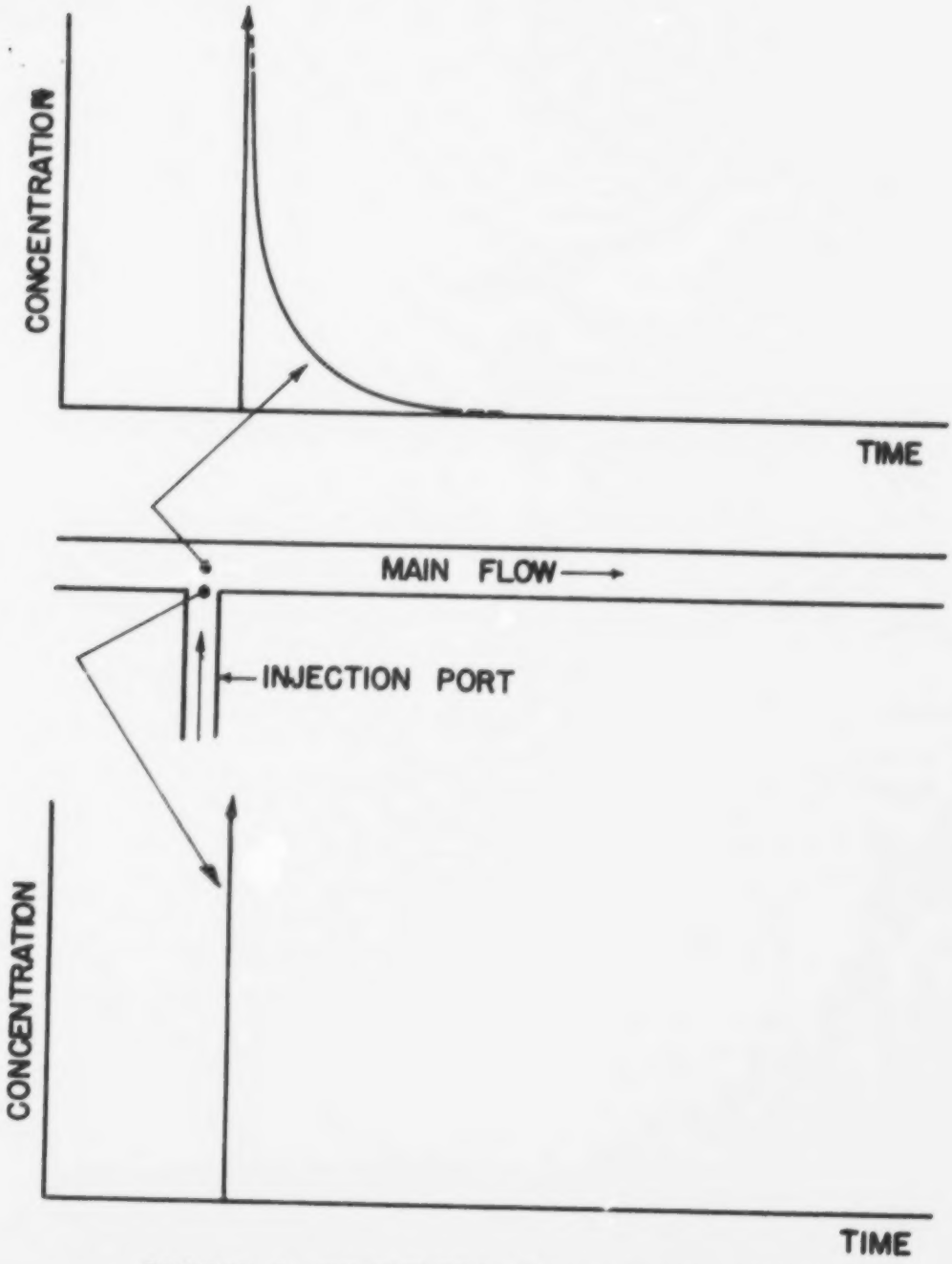


FIGURE 3 CONCENTRATION PROFILES FOR AN INJECTION IMPULSE

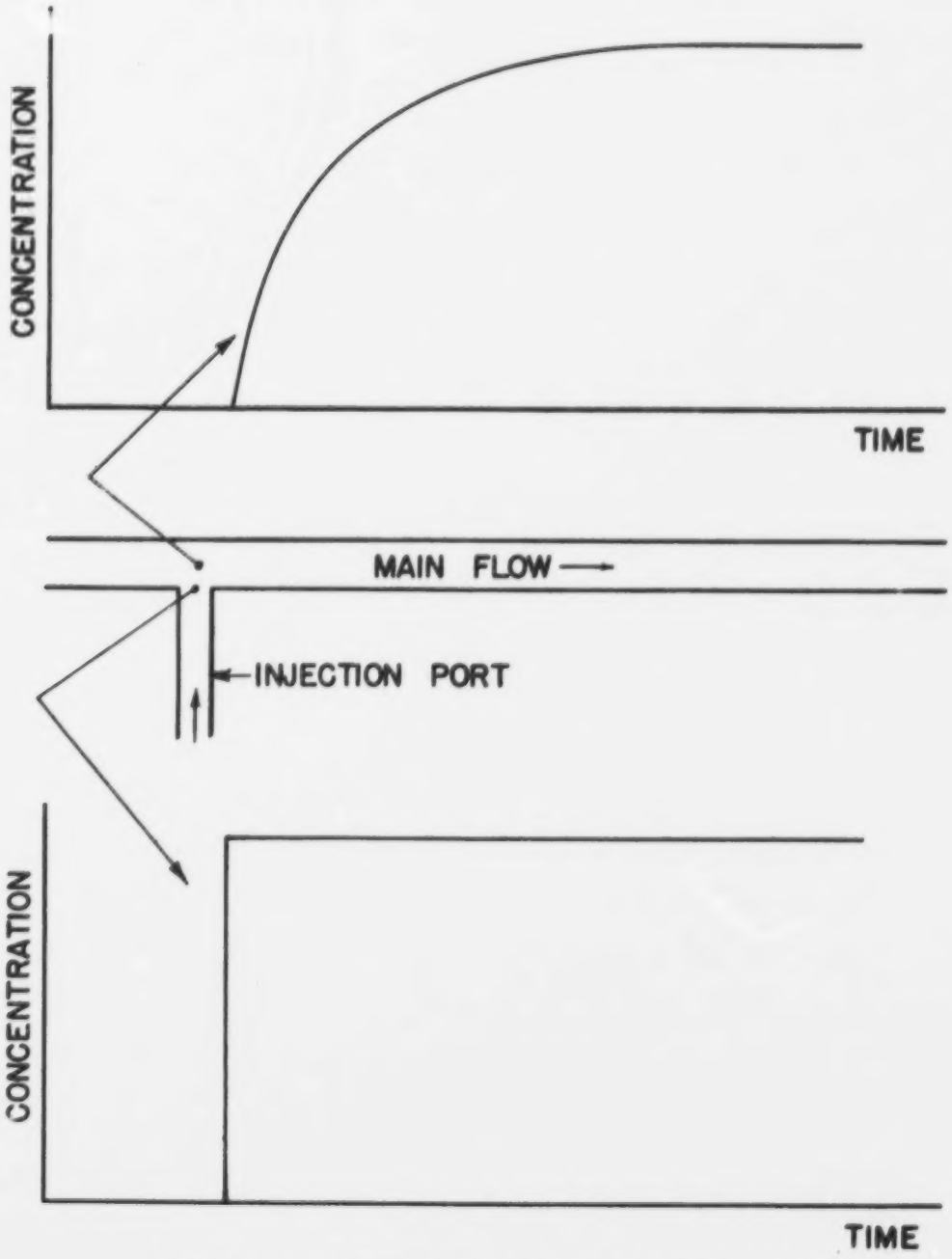


FIGURE 4 CONCENTRATION PROFILES FOR A STEP INJECTION INPUT

the results predicted by the model and the results observed in the system itself. It is quite common to use the sums of the squares of the deviations between the observed and predicted results as a measure of deviation. This is convenient for point data but for continuous information the integral of the squared error is used to measure deviation (13). This measure of deviation, ϕ, is defined as

$$\phi = \int_{t_a}^{t_b} \left[y_o(t) - y_p(t) \right]^2 dt \qquad (45)$$

In equation 45, t is the independent variable and t_a to t_b is the region of interest of the independent variable over which the deviation between $y_o(t)$, the observed results, and $y_p(t)$, the predicted results, is to be computed.

If the physical system under consideration can be tested with an instantaneous injection of tracer, Levenspiel's solution can be used to ascertain the applicability of the one dimensional diffusion model. It is necessary for the method of comparison of the experimental data with the model prediction to indicate how well the model "fits" the system. Only after this question is answered can attention be turned to the problem of finding certain characteristic parameters of the model such as the axial mixing coefficient. Common methods of determining this parameter from second moments, from time above one-half maximum, or from rate of peak decay presuppose that the model is a perfect description of the system. Therefore these methods give no information about the applicability of the model and the values of the parameters of the system are meaningless unless the model fits.

The minimum value of ϕ is a measure of model fit. It is common to call the procedures by which ϕ is minimized the "least squares method". Linear least

squares refers to functions of the independent variable that result in a set of simultaneous equations which are linear in the parameters. Non-linear least squares refers to similar functions which are non-linear in the parameters. The solutions of the non-linear equations cannot be given explicitly and an iterative procedure must be used. It may be easier to minimize ϕ by a direct iterative procedure rather than to solve the non-linear simultaneous equations. Marquardt (18) has reviewed this minimization procedure in some detail and has written a non-linear least squares computer program using the direct iterative approach. This program is available through SHARE (19). In addition to the minimization of ϕ, the non-linear least squares procedure simultaneously gives the best statistical values of the parameters.

Figure 5 qualitatively shows Levenspiel's model compared to a pulse resulting from an instantaneous injection. It can be seen the model does not "fit". The large value of the minimum ϕ that would result from the use of the least squares program gives a quantitative measure of the poor fit. Values of the model parameters for this case would be almost meaningless regardless of the method by which they are computed.

In many cases it is not physically feasible to achieve an instantaneous injection. However, it may be possible to measure the input concentration as a function of time and Clements' solution for an arbitrary input concentration pulse would be applicable.

$$C(x,t) = C_{1\ in}(t) * \left[\frac{x}{t} \sqrt{\frac{1}{4\pi D_L t}} \quad \exp - \frac{(x - ut)^2}{(4D_L t)} \right] \qquad (46)$$

The numerical convolution indicated by the above equation is quite time consuming. In a non-linear least squares computation, which is an iterative

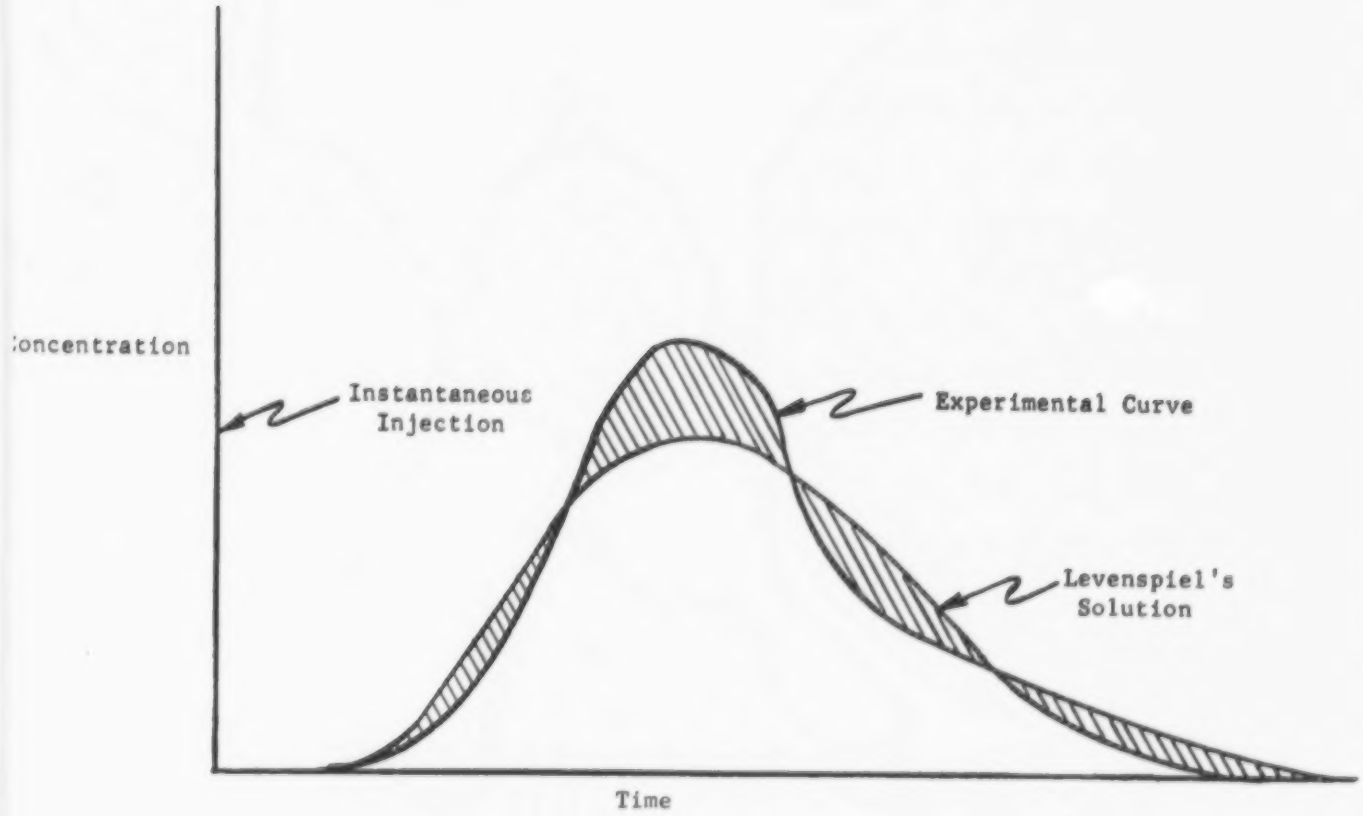


Figure 5

Levenspiel's Solution Compared to an Instantaneous Injection

process, the convolution must be performed a large number of times. These considerations make the direct application of the least squares method in the time domain unattractive. Fortunately, transformation of the model and the data to the frequency domain provides a means of circumventing these difficulties. Hays (10) has shown that ϕ can be written in terms of frequency domain variables as

$$\phi = \frac{1}{\pi} \int_0^\infty \left| Y_o(j\omega) - Y_p(j\omega) \right|^2 d\omega \qquad (47)$$

In this case $Y_p(j\omega)$ is given by Clements' frequency domain solution and $Y_o(j\omega)$ can be obtained from the input and output concentration pulses by the pulse to frequency program. Minimization of ϕ as defined in the frequency domain proceeds in the same manner as discussed above for ϕ defined in the time domain.

AN APPLICATION OF PULSE TESTING TECHNIQUES TO FREQUENCY DOMAIN MODELING

A preliminary study was undertaken (see Hays (10)) to determine the limits of applicability of the one dimensional transport model, equation 1, to flow in a circular pipe. In selecting the testing technique the possibility of attaining an instantaneous injection was considered. If this method were to be employed, then Levenspiel's solution (equation 44) would be applicable. Due to the difficulties of constructing injection equipment to achieve the instantaneous injection required by Levenspiel's solution, the experimental procedure was designed to utilize the arbitrary input pulse - or pulse testing technique. Therefore, the frequency domain solution of Clements (equation 38) and the frequency domain modeling technique were used.

Apparatus

Figure 6 is a schematic of the test apparatus. Tap water was pumped through

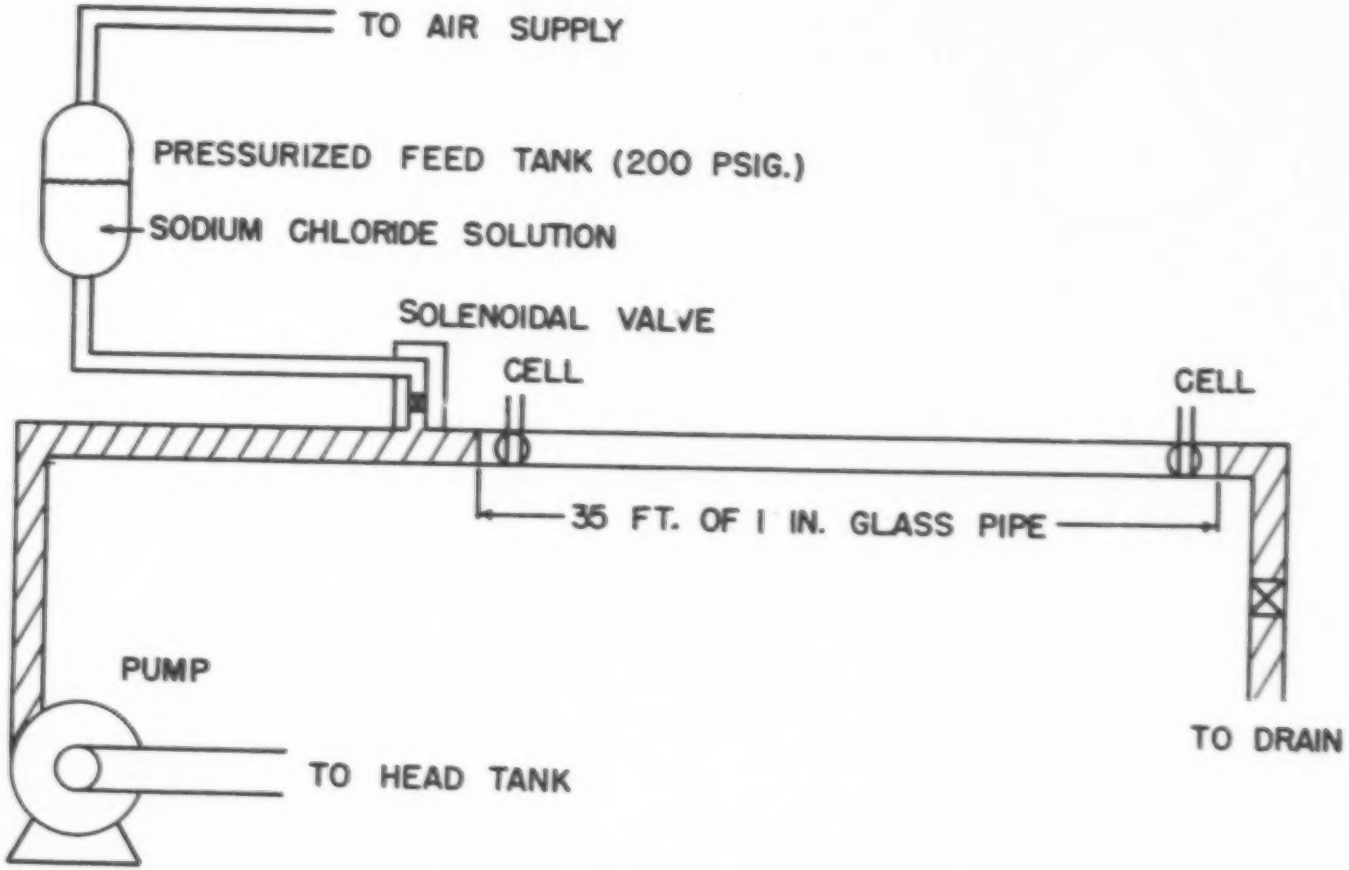


FIGURE 6 SCHEMATIC OF TEST APPARATUS

a 35 foot long one-inch diameter Pyrex pipe test section. The input pulse consisted of aqueous solutions of sodium chloride containing a suspension of carbon black to make the pulse visible in the glass test section. The pulse was injected through a solenoid valve fed from a pressurized tank. The injector was located several feet upstream of the first measuring device to insure cross sectional homogeneity of the pulse when it reached the device. Concentration measurements were made by use of electrical conductivity cells located near the inlet and outlet of the test section. The conductivity-concentration relationship was linear over the range of concentrations investigated. A sine wave generator and a power amplifier were used to generate a 1000 cycle sine wave voltage. The voltage source was connected in series with the cell and a full wave rectifier. The D.C. current furnished by the bridge was sufficient to drive the galvanometers of a model 1406 Honeywell oscillographic recorder without amplification.

Results

The results of this study can be summarized in two graphs. Figure 7 shows a plot of standard error of estimate vs. Reynolds number. The standard error of estimate is a measure of how well the model predicts axial mixing. It can be seen that at high Reynolds numbers the error is of the same order of magnitude as the experimental error, implying a near perfect "fit" in that region. The error increases with decreasing Reynolds number and becomes quite large approaching laminar flow.

Figure 8 shows a plot of Peclet number vs. Reynolds number. Included on this plot are Taylor's (9) experimental points and the theoretically predicted line of Taylor, also, the experimental points of this study and the straight line determined by these points are shown. The theoretically predicted line

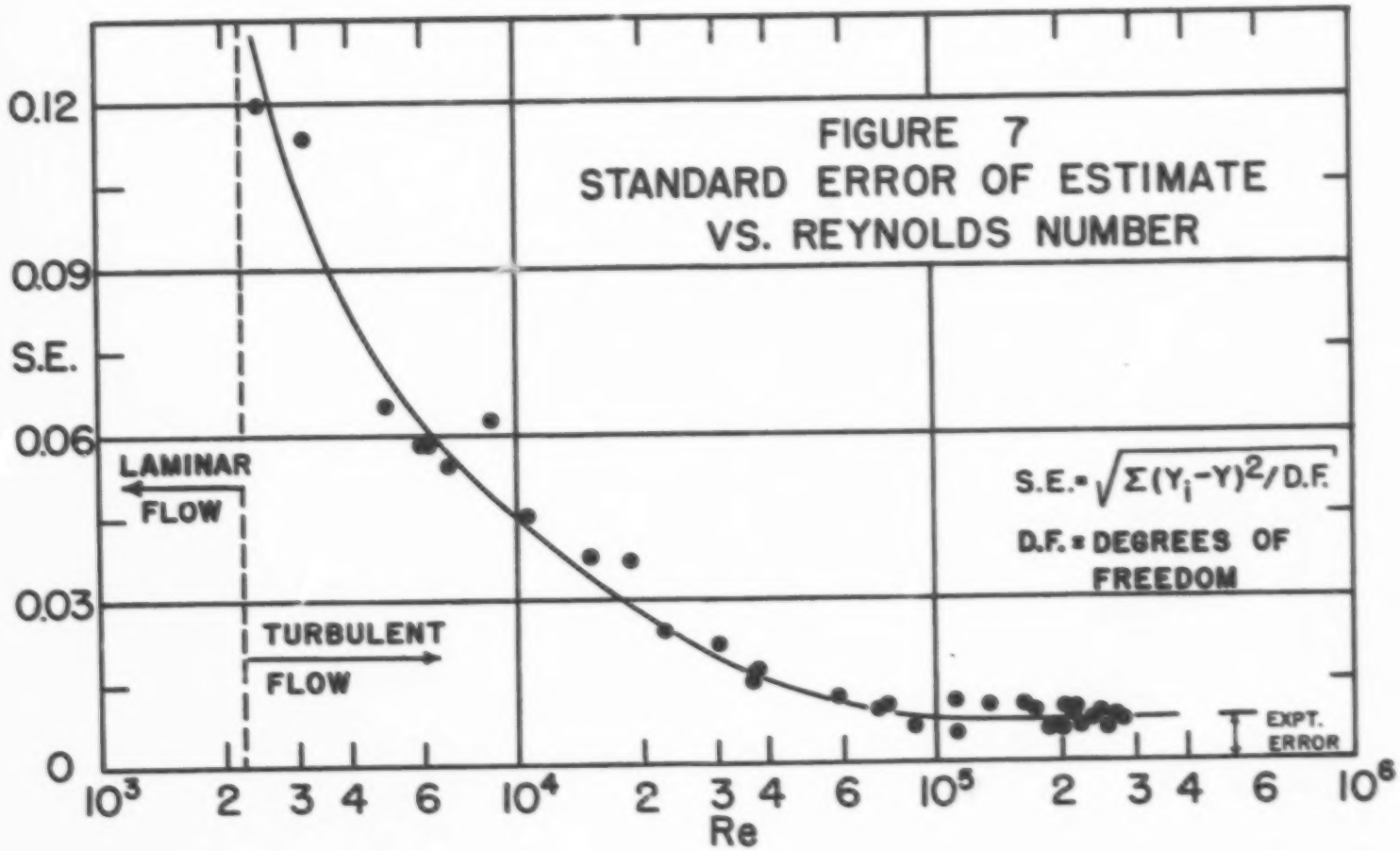


FIGURE 7
STANDARD ERROR OF ESTIMATE
VS. REYNOLDS NUMBER
0.12
0.09
S.E.
0.06
0.03
0
LAMINAR
FLOW
TURBULENT
FLOW
S.E. = √Σ(Yi-Y)²/D.F.
D.F. = DEGREES OF
FREEDOM
EXPT.
ERROR
10³ 2 3 4 6 10⁴ 2 3 4 6 10⁵ 2 3 4 6 10⁶
Re

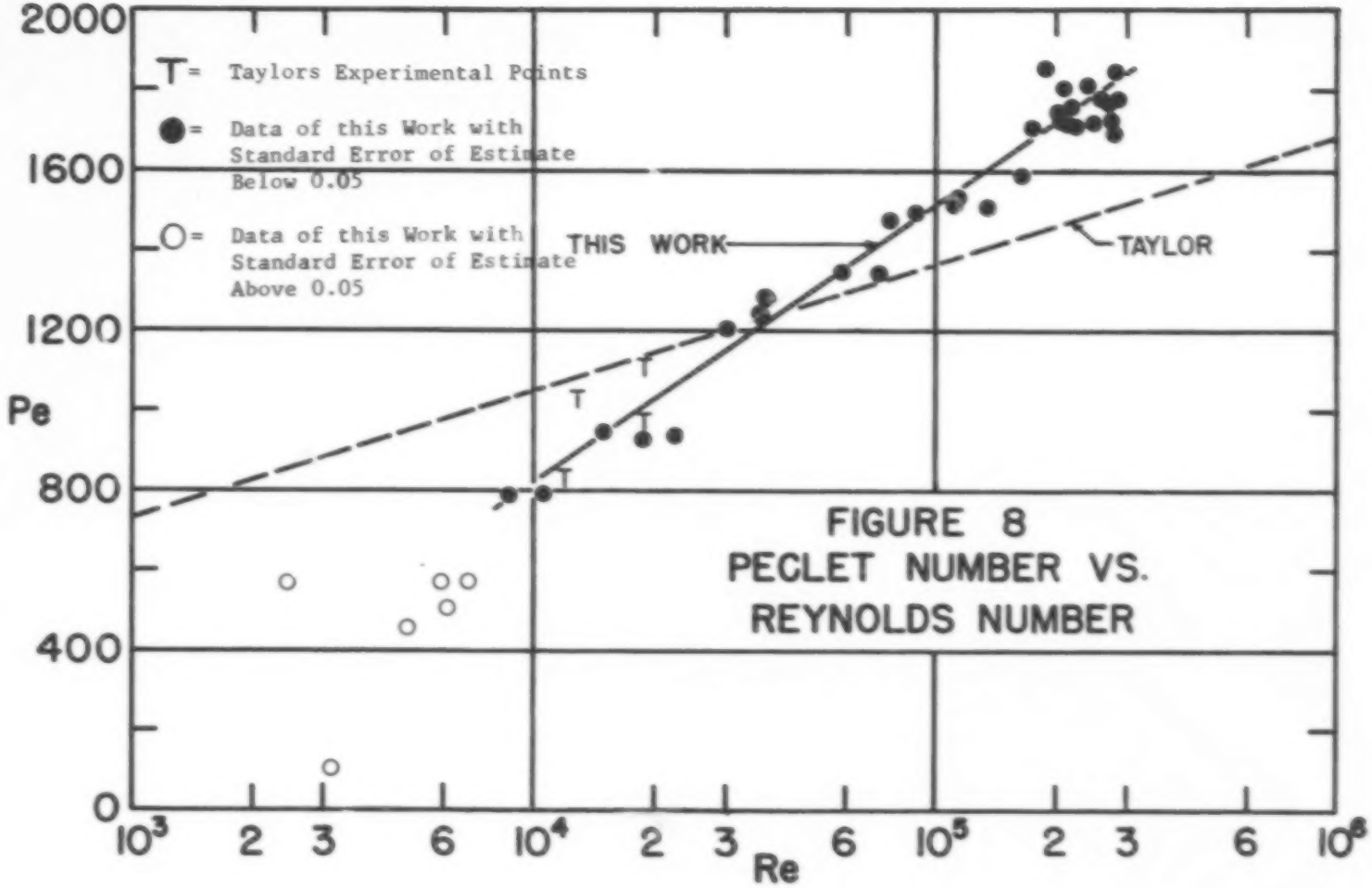


FIGURE 8
PECLET NUMBER VS.
REYNOLDS NUMBER

of Taylor does not agree with the experimental points. It predicts too much axial mixing (a small Peclet number) at high Reynolds numbers, and too little axial mixing (a larger Peclet number) at low Reynolds numbers. The straight line relation of Peclet number and Reynolds number on a semi-log plot, however, is evident. The equation of this line was found to be

$$Pe = -1958 + 694 \log Re$$

while the theoretical equation of Taylor is

$$Pe = -271 + 326 \log Re$$

On the basis of this study alone it would seem premature to suggest that the experimentally determined relationship between Reynolds and Peclet numbers should be used in preference to Taylors expression. Thus, the study should be extended to pipes of other diameters to allow wider variation in the values of the parameters studied. In addition, the effect of the ratio of pulse length to pipe diameter on the standard error of estimate should be investigated.

ACKNOWLEDGEMENT

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NOMENCLATURE

A	Cross Sectional area of pipe, L^2
A,B,C,D	Arbitrary constants defined when used
a,b	Arbitrary quantities defined at time of use
C	Concentration M/L^3
$\bar{C}$	Laplace transform of C
D_L	Longitudinal mixing coefficient, L^2/T
D_x	Mixing in the x direction, L^2/T
D_y	Mixing in the y direction, L^2/T
D_z	Mixing in the z direction, L^2/T
$G(j\omega)$	Fourier transfer function
G(s)	Laplace transfer function
$G(Z, S_n)$	Laplace transfer function
$g(Z, \theta)$	Inversion of $G(Z, S_n)$
g(x,t)	Impulse response
j	Square root of minus one
L	Length of test section, L
$\mathcal{L}$	Laplacian operator
M	Mass of injected tracer, M
M.R.	Magnitude ratio
P.A.	Phase angle
Pe	Peclet number = uL/D_L
Re	Real part of a Fourier transform and Reynolds Number
S.E.	Standard error of estimate
s	Laplace transform variable

S_n	Dimensionless Laplace transform variable
$S_{xn}(\omega)$	Normalized input frequency content
$S_{yn}(\omega)$	Normalized output frequency content
t	Time, T
T	Time constant, T
T_x	Duration of input pulse, T
T_y	Duration of output pulse, T
u	Velocity, L/T
V	Volume of test section, or tank volume, L^3
x	Length coordinate L
$X(j\omega)$	Fourier transform of x(t)
X(s)	Laplace transform of x(t)
x(t)	Input
$Y(j\omega)$	Fourier transform of y(t)
y_o	Observed or experimentally measured value of a dependent variable
y_p	Predicted value of a dependent variable
Y(s)	Laplace transform of y(t)
y(t)	Output
Z	Dimensionless length = X/L
z	Independent space variable, L
∇^2	Laplacian operator = $\frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2}$
θ	Dimensionless time = ut/L
ϕ	Integral of the squared error
ω	Frequency
ω_n	Nondimensional frequency

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